

MANY-PARTICLE LIMITS AND NON-CONVERGENCE OF DISLOCATION WALL PILE-UPS

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ABSTRACT. The starting point of our analysis is a class of one-dimensional interacting particle systems with two species. The particles are confined to an interval and exert a nonlocal, repelling force on each other, resulting in a nontrivial equilibrium configuration. This class of particle systems covers the setting of pile-ups of dislocation walls, which is an idealised setup for studying the microscopic origin of several dislocation density models in the literature. Such density models are used to construct constitutive relations in plasticity models.

Our aim is to pass to the many-particle limit. The main challenge is the combination of the nonlocal nature of the interactions, the singularity of the interaction potential between particles of the same type, the non-convexity of the the interaction potential between particles of the opposite type, and the interplay between the length-scale of the domain with the length-scale ℓ_n of the decay of the interaction potential. Our main results are the Γ -convergence of the energy of the particle positions, the evolutionary convergence of the related gradient flows for ℓ_n sufficiently large, and the non-convergence of the gradient flows for ℓ_n sufficiently small.

Keywords: Particle system, Discrete-to-continuum asymptotics, Γ -convergence, Gradient flows.
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1. INTRODUCTION

Plasticity of metals is facilitated by many *dislocations* (i.e., line defects in the crystallographic lattice) interacting on a small length-scale. Since it is undesirable and computationally heavy to model plasticity by keeping track of individual dislocations, there is a large community which develops models for the dislocation density; see, e.g., [GB99, GCZ03, HZG07, KHG15] for several such models. However, due to the complexity of the dislocation interactions, these models lack a mathematically precise connection with the dislocation interactions on the microscale. In this paper we seek such a connection for a family of simplified models for interacting dislocations, parametrised by two parameters. We both prove such connections for certain scaling regimes of the parameters (Theorem 1.1 and Theorem 6.7), and identify *non-convergence* in other scaling regimes (Proposition 1.2 and Proposition 7.2).

The simplified model for the interacting dislocations which we consider in this paper is a one-dimensional interacting particle system with two species (see §1.1). Interacting particle systems with multiple species are of rapidly increasing interest; see, e.g., [CXZ16, DFF13, BBP16, EFK16] and the references therein for applications to dislocation networks, cellular aggregation, granular media, pedestrian movement, opinion formation and predator-pray models. A common challenge in these particle systems is the passage to the many-particle limit. The complexity of this limit passage lies in the high sensitivity of the particle system on the type of interactions between particles of the same species and the type of interactions between particles of different species. Our aim is therefore to impose minimal assumptions on the interaction potential.

1.1. The particle system. The starting point of our analysis is a more general version of the one-dimensional particle system posed in [DPG15]. In §2 we describe how the system in [DPG15] models interacting dislocations. Here, the state of the particle system is characterised by a one-dimensional chain of $n^+ \in \mathbb{N}$ positive particles and $n^- \in \mathbb{N}$ negative particles with positions

$$x^{n,\pm} := (x_1^\pm, \dots, x_{n^\pm}^\pm)^T \in \Omega_n^\pm := \{y \in \mathbb{R}^{n^\pm} : 0 \leq y_1 < \dots < y_{n^\pm} \leq 1\}, \quad (1)$$

where $n := n^+ + n^-$ is the total number of particles. Figure 1 illustrates an example.

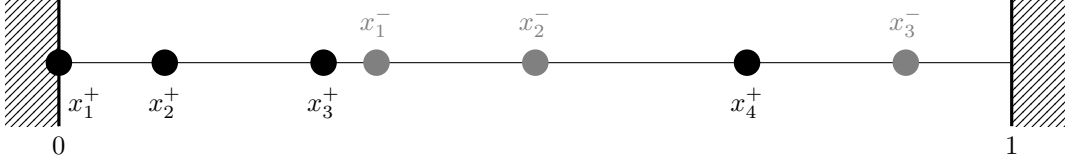


FIGURE 1. Example of $x^{n,+}$ (black) and $x^{n,-}$ (gray) for $n^+ = 4$ and $n^- = 3$.

We consider the energy $E_n : \Omega_n^+ \times \Omega_n^- \rightarrow \mathbb{R}$ given by

$$\begin{aligned}
 E_n(x^{n,+}, x^{n,-}) = & \frac{1}{n^2} \sum_{i=1}^{n^+} \sum_{j=1}^{i-1} \alpha_n V(\alpha_n(x_i^+ - x_j^+)) + \frac{1}{n^2} \sum_{i=1}^{n^-} \sum_{j=1}^{i-1} \alpha_n V(\alpha_n(x_i^- - x_j^-)) \\
 & + \frac{1}{n^2} \sum_{i=1}^{n^+} \sum_{j=1}^{n^-} \alpha_n W(\alpha_n(x_i^+ - x_j^-)) + \gamma_n^2 \frac{1}{n} \sum_{i=1}^{n^+} x_i^+ + \gamma_n^2 \frac{1}{n} \sum_{i=1}^{n^-} (1 - x_i^-). \quad (2)
 \end{aligned}$$

The parameter $\gamma_n \geq 0$ regulates the strength of the affine external potential (which models a constant applied force on the particles), which favours the positive particles to cluster at the left barrier at $x = 0$ and the negative particles to cluster at the right barrier at $x = 1$. The parameter $\alpha_n = \ell_n^{-1} > 0$ is the inverse of the length-scale of the decay of the interactions between particles. The corresponding interaction potential for particles of the same type is given by $V : \mathbb{R} \rightarrow (-\infty, \infty]$, and $W : \mathbb{R} \rightarrow \mathbb{R}$ denotes the interaction potential for particles of opposite type. Figure 2 illustrates prototypical examples for V and W . Minimal assumption on V and W are that $W \in L^\infty(\mathbb{R})$, and V is bounded from below on \mathbb{R} , bounded from above on compact sets of $\mathbb{R} \setminus \{0\}$ while $V(r) \rightarrow \infty$ as $r \rightarrow 0$. The singularity of V at 0 and the boundedness properties of V and W prevent the particles from clustering, which therefore results in a nontrivial interplay with the external loading term. We leave the precise assumptions on V and W to Theorem 1.1 and Theorem 6.7.

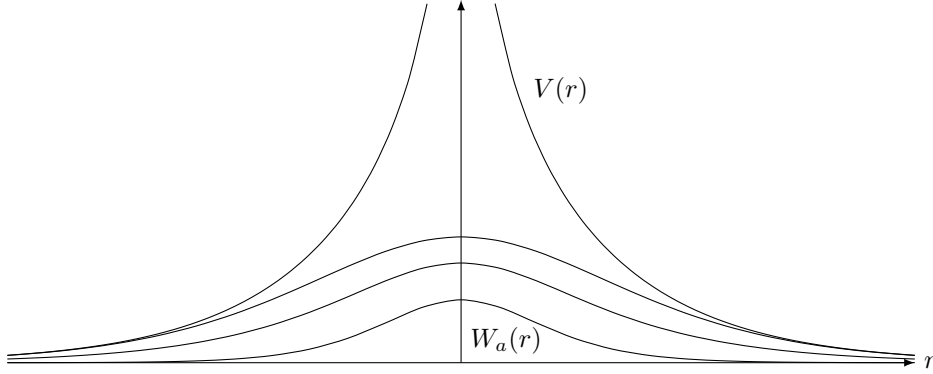


FIGURE 2. Plots of V and three choices for W (labelled W_a for $a = 0, \frac{1}{2}, 1$, from bottom to top) corresponding to dislocation walls (see (11) and (12) for the precise expressions).

1.2. The parameters α_n and γ_n in the single-species case. Even in the single-species case ($n^- = 0$), the asymptotic behaviour of the parameters α_n and γ_n as $n \rightarrow \infty$ is crucial for the features of the many-particle limit. These many particle-limits were established first in [GPPS13] on the half-infinite domain $[0, \infty)$ with $\gamma_n = 1$ to keep the particles confined. The corresponding

energy reads

$$\tilde{E}_n(x^n) = \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^{i-1} \alpha_n V(\alpha_n(x_i - x_j)) + \frac{1}{n} \sum_{i=1}^n x_i.$$

Depending on the asymptotic behaviour of α_n , five different limiting energies for the particle density were derived. Two of them are characterised by $\alpha_n \rightarrow \alpha > 0$ and $\frac{1}{n}\alpha_n \rightarrow \alpha > 0$ as $n \rightarrow \infty$, and the other three treat the case in which α_n is either asymptotically larger or smaller than any of these two limiting cases.

Many particle systems in the literature fit to $\alpha_n \rightarrow \alpha > 0$, which corresponds to a setting where the length-scale of V is proportional to the length-scale of the support of the particle density. In particular, if the particles remain in a bounded set, then \tilde{E}_n is independent of the tails of V . The many-particle limit of such systems is studied extensively; see, e.g., [Sch96, PS14, Due16, Hau09, MPS14, GLP10, CP16] for a wide range of potentials, corrector estimates, gradient flows, and higher dimensional domains.

Another important class of particle systems corresponding to $\frac{1}{n}\alpha_n \rightarrow \alpha > 0$ is given by atoms interacting by a Lennard-Jones potential, and is therefore studied in many different contexts [Hud13, HO14, BG04, BLBL07, HHvM16, FIM09]. One characteristic of the related particle system is that the length-scale of V is proportional to the length-scale of neighbouring particles, which typically scales as $\frac{1}{n}$ times the length-scale of the support of the particle density. As a result, \tilde{E}_n is hardly sensitive to changes in the singularity of V at zero, while the tail behaviour of V shapes the limiting energy. Consequently, the proofs that establish the many-particle limit in this scaling regimes differ completely from the regime in which $\alpha_n \rightarrow \alpha > 0$.

The limiting energy of the intermediate regime $1 \ll \alpha_n \ll n$ has the porous medium equation as its gradient flow (see [Oel90] for V regular enough). The minimisers exhibits intricate boundary layers [HCO10, GvMPS16], and again the proof for the many-particle limit differs substantially. A more detailed discussion on all scaling regimes of α_n and their connection is given in [GPPS13, SPPG14].

In [vMMP14] the single-type scenario in [GPPS13] is extended by considering finite domains. The corresponding energy is given by E_n as in (2) with $n^- = 0$. The main result in [vMMP14] is that the asymptotic behaviours of α_n and γ_n can be treated independently in the many-particle limit, given a convenient rescaling of the particle positions (and $\frac{1}{n}\alpha_n$ bounded). Consequently, the asymptotic behaviour of α_n has the same effect on the interactions in the limit $n \rightarrow \infty$ as in [GPPS13]. Moreover, the asymptotic behaviour of γ_n determines whether the particles in the limit $n \rightarrow \infty$ are confined by either the finite domain ($\gamma_n \rightarrow 0$), the external force ($\gamma_n \rightarrow \infty$), or both effects ($\gamma_n \rightarrow \gamma > 0$).

1.3. Connection to the literature on multiple-species models. While there are many results in the literature on many-particle limits of E_n as in (2) for the single-type scenario (see §1.2), few results exist on many-particle limits of multiple specie models. In [DFF16, Zin16] a stability result is proven for solutions of the continuum gradient flow related to $\alpha_n \rightarrow \alpha > 0$. Since these results require V to be regular (in particular $V(0) < \infty$), the discrete gradient flow satisfies the same weak equation as the continuum gradient flow, and thus the stability result includes the many particle limit. Since we wish to include potentials V that are singular at 0, we need to seek other proof methods.

In [CXZ16] the upscaling of many dislocation dipoles (pairs of positive and negative dislocations) is studied in a dynamical setting with formal asymptotic techniques. While their setting relates to ours by setting $V = -\log$ and $W_n \rightarrow -V$, the unboundedness of $W_n(0)$ as $n \rightarrow \infty$ results in intricate effects (e.g., a fast time-scale describing dipole formation) which we do not address here.

Therefore, in the proof of Theorem 1.1, we rely on the methods developed in the literature of single-type scenarios. However, in the cases when $\alpha_n \rightarrow \infty$, we need to develop a new proof strategy, because the techniques in [BG04] and [GPPS13] do not apply. This strategy seem flexible for extensions to higher dimensions, and is therefore one of the main contributions of this paper.

1.4. Theorem 1.1: Γ -convergence of E_n . Similarly to [vMMP14], we identify the vectors $x^{n,\pm}$ by their empirical distribution

$$\mu_n^\pm := \frac{1}{n} \sum_{j=1}^{n^\pm} \delta_{x_j^\pm}, \quad (3)$$

which have total mass $n^\pm/n \in [0, 1]$. We say that μ_n^\pm converges in the *narrow topology* to a measure μ^\pm if

$$\int_0^1 \varphi d\mu_n^\pm \xrightarrow{n \rightarrow \infty} \int_0^1 \varphi d\mu^\pm \quad \text{for all } \varphi \in C([0, 1]), \quad (4)$$

where the integrals are taken over the closed interval $[0, 1]$.

To state the main result (Theorem 1.1) we extend E_n to apply to measures by setting

$$E_n(\mu^+, \mu^-) = \begin{cases} E_n(x^{n,+}, x^{n,-}), & \text{if } \mu^\pm = \frac{1}{n} \sum_{j=1}^{n^\pm} \delta_{x_j^\pm}, \\ \infty, & \text{otherwise.} \end{cases}$$

Theorem 1.1 (Γ -convergence). *Let $\gamma_n \rightarrow \gamma \in [0, \infty)$ and $\alpha_n > 0$ be such that either $\alpha_n \rightarrow \alpha$, $1 \ll \alpha_n \ll n$ or $\frac{1}{n}\alpha_n \rightarrow \alpha$ as $n \rightarrow \infty$ for some $\alpha \in (0, \infty)$. Depending on the scaling regime of α_n , let V , W and $E^{(\text{int})}$ be as in Table 1. Then E_n Γ -converges with respect to the narrow topology to*

$$E(\mu^+, \mu^-) := E^{(\text{int})}(\mu^+, \mu^-) + \gamma^2 \int_0^1 x d\mu^+(x) + \gamma^2 \int_0^1 (1-x) d\mu^-(x).$$

1.5. Comments on Theorem 1.1. Compactness. Compactness is for free since the space of non-negative Borel measures on $[0, 1]$ with total variation bounded by 1 is compact with respect to the narrow topology.

Assumptions on V and W . The assumptions on V and W are such that the case of dislocation walls in §2 is covered for all scaling regimes of α_n as in Table 1. Moreover, the assumptions on V extend the setting in [GPPS13]. In particular, we relax convexity of $V|_{(0,\infty)}$.

Proof strategy. In all scaling regimes of α_n , we pass to the limit $n \rightarrow \infty$ in the setting of measures (3). While this is a common approach when $\alpha_n \rightarrow \alpha > 0$, most literature on many-particle limits for $\frac{1}{n}\alpha_n \rightarrow \alpha > 0$ deals with the displacement function $u_n : [0, 1] \rightarrow [0, 1]$, which

Regime	V, W satisfy	$E^{(\text{int})}(\mu^+, \mu^-)$
$\alpha_n \rightarrow \alpha$	Assumption 4.1	$\frac{1}{2} \iint_{[0,1]^2} \alpha V(\alpha(x-y)) d(\mu^+ \otimes \mu^+ + \mu^- \otimes \mu^-)(x, y)$ $+ \iint_{[0,1]^2} \alpha W(\alpha(x-y)) d(\mu^+ \otimes \mu^-)(x, y)$
$1 \ll \alpha_n \ll n$	Assumption 4.4	$\left(\int_0^\infty V \right) \int_0^1 (\rho^+(x)^2 + \rho^-(x)^2) dx$ $+ \left(\int_0^\infty W \right) \int_0^1 2\rho^+(x)\rho^-(x) dx$
$\frac{\alpha_n}{n} \rightarrow \alpha$	Assumption 4.7	$\int_0^1 \psi(\rho^+(x), \rho^-(x)) dx,$

TABLE 1. Expressions for $E^{(\text{int})}$, the interaction part of the limit energy in Theorem 1.1. For $\alpha_n \gg 1$ the expressions are valid when μ^+ and μ^- are absolutely continuous (see (16)) with density $\rho^+, \rho^- \in L^2(0, 1)$ respectively; otherwise $E^{(\text{int})}(\mu^+, \mu^-) = \infty$. The function $\psi \in C([0, \infty)^2)$ is implicitly determined as a limit of cell-problems (28a).

maps the reference lattice of equispaced points $\frac{1}{n}, \frac{2}{n}, \dots, 1$ to x_1, x_2, \dots, x_n . In this approach, the argument for the many-particle limit relies on the ordering of the particles by

$$u'_n(s) = n(x_{i+1} - x_i) \quad \text{with } i \text{ such that } x_i < s \leq x_{i+1}. \quad (5)$$

While we assume x_n^+ and x_n^- to be ordered vectors, there is no natural ordering in the combined vector x^n , and it is therefore not clear how to write $x_i^+ - x_j^-$ conveniently in terms of u_n^+ and u_n^- . Moreover, while the expressions for $E^{(\text{int})}$ as in Table 1 describing the interactions between particles of the same type can be conveniently cast in terms of a displacement map u^\pm [GPPS13], it is unclear how the terms describing the interactions between particles of opposite type can be written in terms of u^+ and u^- (except for the case $\alpha_n \rightarrow \alpha > 0$). Nonetheless, our proof is much inspired by [BG04], in which E_n is approximated by a sum of cell problems.

As a consequence of using the setting of measures, where the ordering of the particles is not inherently used, a generalisation to higher dimensions is within reach. We keep the present setting one-dimensional to simplify the arguments and to cover the model of dislocations described in §2.

Other scaling regimes. Several scaling regimes of the parameters γ_n and α_n are excluded in Theorem 1.1. We comment on the meaning of these scaling regimes and the corresponding many-particle limit of E_n :

- the scaling regime $\gamma_n \rightarrow \infty$ corresponds to a scenario in which the external forcing term is large enough to separate the positive particles from the negative particles into pile-ups at the barriers, whose length scale is asymptotically smaller than L_n . Consequently, the scaling introduced in (1) does not conserve information on the particle distribution in the limit $n \rightarrow \infty$. In §5, we introduce a different scaling (equivalent to the scaling in [GPPS13]), and prove a Γ -convergence result on the corresponding energy (see Theorem 5.2). The Γ -limit \tilde{E} decouples the dependence on μ^+ and μ^- , i.e.

$$\tilde{E}(\mu^+, \mu^-) = \tilde{E}^+(\mu^+) + \tilde{E}^-(\mu^-), \quad (6)$$

where \tilde{E}^\pm are equivalent to the energy studied in [GPPS13] except for μ^\pm not having unit mass;

- the scaling regime $\alpha_n \rightarrow 0$ treats the case in which all particle interactions are given by the asymptotic behaviour of the singularity of V at 0. Consequently, any useful scaling of the energy depends on the type of singularity. For a logarithmic singularity of V , it is shown in [vMMP14] that the scaling

$$\frac{1}{\alpha_n} E_n(x^{n,+}, x^{n,-}) + \frac{(n^+)^2 + (n^-)^2 - n}{2n^2} \log \alpha_n$$

results in a non-trivial Γ -limit whenever $n^- = 0$. It is easy to extend this result to the case of mixed particles under the assumption that W is continuous at 0. Indeed, since $|x_i^+ - x_j^-| \leq 1$, it holds that

$$W(\alpha_n(x_i^+ - x_j^-)) \xrightarrow{n \rightarrow \infty} W(0)$$

uniformly in i and j . Hence, the interactions between positive and negative particles are a continuous perturbation to the energy, and their contribution converges to a constant in the Γ -limit. Thus, the Γ -limit effectively decouples as in (6).

Other types of singularities of V need to be dealt with in a slightly different way. Consider for example $V(r) = r^{-s}$ with $0 < s < 1$. Then, the right scaling of the energy is $\alpha_n^{s-1} E_n(x^{n,+}, x^{n,-})$, and the contribution of the interactions between particles of opposite type vanishes in the limit $n \rightarrow \infty$.

- the scaling regime $\alpha_n \gg n$ describes the opposite effect of $\alpha_n \rightarrow 0$, i.e., all particle interactions are described by the tail-behaviour of V instead. Again, any useful scaling of the energy depends on a detailed description of these tails. For example, V and W given by (11) and (12) have tails which decay exponentially fast. To preserve the effect of the interactions in E_n in the limit $n \rightarrow \infty$, we need an exponentially large prefactor to the energy. For $n^- = 0$ this regime is treated in full detail in [vMMP14].

1.6. Asymptotic behaviour of the gradient flows of E_n . To treat the many-particle limit of the gradient flow dynamics, we introduce an alternative representation for the particle positions. Given n^\pm and $x^{n,\pm}$, we collect the particle positions x_i^\pm in an ordered vector $x^n \in [0, 1]^n$, i.e., $0 \leq x_1 \leq \dots \leq x_n \leq 1$, and keep track of their sign by a vector $b^n := (b_1, \dots, b_n) \in \{-1, 1\}^n$. There is an obvious isomorphism between x^n, b^n and $x^{n,\pm}$, and thus we switch between both descriptions whenever convenient.

The gradient flow of E_n is given by

$$\begin{cases} \frac{d}{dt}x^n(t) = -n\nabla E_n(x^n(t)), & t > 0, \\ x^n(0) = x_\circ^n. \end{cases} \quad (7)$$

where $x_\circ^{n,\pm} \in \Omega_n^\pm$ is a suitable initial condition. Given Theorem 1.1, it is natural to investigate the possibility to pass to the limit $n \rightarrow \infty$ in (7). Such limit passage is obtained in [vMM14] in the single-type case with $V|_{(0,\infty)}$ convex. However, since we consider non-convex W , we need to resort to different methods. To this aim, we discuss several evolutionary convergence techniques in the literature:

- (1) if E_n is λ -convex for an n -independent λ , then the theory in [AGS08, Chap. 4] applies, and the evolutionary convergence method in [DS10, Thm. 2.17] is within reach. We show in §6 that, under mild conditions on V and W , E_n is λ_n -convex with $\mathcal{O}(-\lambda_n) = \alpha_n^3$. Then, in the scaling regime $\alpha_n \rightarrow \alpha > 0$, we show how (7) fits to [DS10, Thm. 2.17]. Theorem 6.7 states the evolutionary convergence result of (7);
- (2) the general framework by [SS04] requires a characterisation of slopes or upper gradients of E_n and E with a related liminf-inequality. This characterisation is difficult to prove, except for the λ -convex case (see [Ort05]), which is considered above;
- (3) if $xV'(x)$ is bounded and $\alpha_n \rightarrow \alpha > 0$, then Schochet's symmetrisation argument in [Sch96] can be used to pass to the limit in the weak form of (7). We apply this method at the end of §6 to describe the limiting gradient flow by a PDE (see (8));
- (4) the scaling regimes $1 \ll \alpha_n \ll n$ and $\frac{1}{n}\alpha_n \rightarrow \alpha > 0$ are treated in [Oel90] for the single-type case with strong regularity conditions on V , including $V(0) < \infty$. The proof method appears difficult to extend to unbounded V , let alone the extension to multiple species.

Using the first method listed above, we prove evolutionary convergence of (7) in Theorem 6.7 in the scaling regime $\alpha_n \rightarrow \alpha > 0$. The limiting gradient flow for $\alpha = 1$ is given by

$$\begin{cases} \frac{\partial \mu^+}{\partial t} = (\mu^+ [(V_\alpha * \mu^+)' + (W_\alpha * \mu_n^-)' + \gamma^2])' & \text{in } \mathcal{D}'((0, \infty) \times (0, 1)), \\ \frac{\partial \mu^-}{\partial t} = (\mu^- [(V_\alpha * \mu^-)' + (W_\alpha * \mu_n^+)' - \gamma^2])' & \text{in } \mathcal{D}'((0, \infty) \times (0, 1)), \end{cases} \quad (8)$$

where \mathcal{D}' denotes the space of distributions on the time-space product space, and $V_\alpha := \alpha V(\alpha \cdot)$ and $W_\alpha := \alpha W(\alpha \cdot)$. The coupled system of continuity equations in (8) is similar to those studied in [DFF16, Zin16] for regular V .

In the scaling regimes where $\alpha_n \rightarrow \infty$, the λ -convexity property of E_n vanishes in the limit $n \rightarrow \infty$, and our proof method of Theorem 6.7 breaks down. To get insight in the solution of the gradient flow (7) for large n , we extend in §7 the numerical simulations of [DPG15] to larger values of n and different values of α_n . We put $\gamma_n = 0$, and take as initial condition a *fully separated* state, i.e.,

$$0 = x_1^+ < \dots < x_{n^+}^+ < x_1^- < \dots < x_{n^-}^- = 1. \quad (9)$$

This setup fits in the framework of dislocations to *interlacing*, which was first considered by [Hea59]. The question is whether the particles remain fully separated during the gradient flow dynamics, and if not, to which extend they ‘interlace’, i.e., the number of particle that swap position.

For V and W as in (11) and (12), the simulations in §7.1 suggest that in the scaling regime $\frac{1}{n}\alpha_n \rightarrow \alpha > 0$ there is a critical value of α beyond which there exist local minima of E_n for n large enough which exhibit full separation (9). In §7.2 we prove the existence of such minimisers

(Proposition 1.2). The idea behind the proof is that for increasing α_n , the interaction forces between particles of the same type becomes smaller, whereas the force needed to push $x_{n^+}^+$ beyond x_1^- becomes larger.

Proposition 1.2. *Let E_n be as in (2) with $\gamma_n = 0$, $\frac{1}{n}\alpha_n = \alpha > 0$, and V and W as in (11) and (12). If α large enough, then for all $n^\pm \geq 2$ the energy E_n admits a local minimiser which is fully separated (see (9)).*

However, at the ‘continuum equivalent’ of the local minimiser in Proposition 1.2 for $n^+ = n^- = \frac{n}{2}$ given by

$$\rho_{\text{sep}}^+(x) := \begin{cases} 1 & x < \frac{1}{2} \\ 0 & x > \frac{1}{2} \end{cases}, \quad \rho_{\text{sep}}^-(x) := \begin{cases} 0 & x < \frac{1}{2} \\ 1 & x > \frac{1}{2} \end{cases}, \quad (10)$$

the Γ -limit E has infinite slope (Proposition 1.2), which would imply that the evolutionary limit of (7) in the scaling regime $\frac{1}{n}\alpha_n \rightarrow \alpha$ with α large enough, if it exists, is *not* given by the Wasserstein gradient flow of E . This reasoning relies on the conjecture that the local minimisers of Proposition 1.2 converge to (10) as $n \rightarrow \infty$ with $n^+ = n^- = \frac{n}{2}$. This conjecture is based on the numerical results in §7.2 listed in Table 5.

Coming back to the criticality of some $\alpha > 0$ in the scaling regime $\frac{1}{n}\alpha_n \rightarrow \alpha > 0$, the numerical results for $\alpha = \frac{1}{2}$ in Table 6 in §7.1 suggest that $x^{n,\pm}(t)$ converges in time to a ‘mixed state’, which on the continuum scale reads as $\rho_{\text{mix}}^+(x) := \frac{1}{2} =: \rho_{\text{mix}}^-(x)$. This observation was also made in [DPG15] for large values of n and for $\alpha_n = C\sqrt{n}$ with C fixed. However, both findings are not very quantitative, and thus the asymptotic behaviour for large n and $1 \ll \alpha_n \ll n$ remains illusive.

1.7. Discussion and conclusion. Motivated by missing rigorous micro-to-macro connections for dislocation density models, we consider a class of interacting particle system (given by the energy E_n (2)) consisting of two species, which is also related to other applications [DFF13, BBP16, EFK16]. For the physically interesting scaling regimes of the parameters α_n and γ_n , we prove that E_n Γ -converges to E (Theorem 1.1). Our proof method is novel and suited for extension to higher spatial dimensions. Regarding the gradient flows of E_n , we prove evolutionary convergence (Theorem 6.7) for the scaling regime $\alpha_n \rightarrow \alpha > 0$ as $n \rightarrow \infty$ in which the nonlocality of the interactions is preserved in the limiting gradient flow (8). However, in the scaling regimes where the limiting energy becomes local (see Table 1), the existence of evolutionary convergence is far from obvious, because the nonconvexity of the interactions may create local minima in E_n (Proposition 1.2) which are seemingly not preserved by the limiting *local* energy (see Proposition 7.2 and Table 5 in §7.1).

For more complex multi-species interacting particle systems (for instance, in higher-spatial dimensions and more complex interactions), our findings therefore imply that it may be possible to prove a Γ -convergence result (and hence convergence of global minimisers), but that there may not be any evolutionary convergence result in the sense of Theorem 6.7. This adds to the findings of [CXZ16] that for n -dependent W_n which become singular in the limit, the limiting gradient flow (if it exists) is much more subtle than the (Wasserstein) gradient flow of the limiting energy E , and may not be expressed in terms of the dislocation densities alone (in addition, one may need internal variables accounting for microstructures such as dipoles). For the current dislocation density models mentioned in the introduction, which are stated in terms of the dislocation densities alone, this statement implies that it is not clear at all whether there exists a precise micro-to-macro connection between these models and the underlying dynamics of individual dislocations. This doubt on the existence of micro-to-macro connections leads to three kinds of future challenges on multi-species particle systems:

- Under which geometric restrictions on the particle system does evolutionary convergence hold in the sense of Theorem 6.7?
- What kind of microscopic particle configurations lead to a *different* evolution of the macroscopic particle density than predicted by the continuum models in the literature?

- If evolutionary convergence in the sense of Theorem 6.7 does not hold for a certain interacting particle system, then can we develop an alternative, satisfactory mathematical statement for ‘evolutionary convergence’?

In a forthcoming paper we give an answer to the first two questions for the celebrated two-species dislocation density model in [GB99]. The third question remains open.

The remainder of the paper is organised as follows. In §2 we show how E_n captures the setting of dislocation walls, and how the parameters α_n and γ_n can be computed from physical quantities. In §3 we introduce the mathematical framework. In §4 we prove Theorem 1.1. In §5 we extend Theorem 1.1 to the case $\gamma_n \rightarrow \infty$. In §6 we prove the evolutionary convergence result (Theorem 6.7) for the gradient flow (7) in the case $\alpha_n \rightarrow \alpha > 0$. In §7 we rely on both analysis and numerical observations to give a convincing argument that the n -dependent gradient flows (7) in the case $\frac{1}{n}\alpha_n \rightarrow \alpha$ for α large enough do not converge to the (Wasserstein) gradient flow of the Γ -limit \bar{E} . In the appendices we perform those parts of the proofs in this paper that are computationally heavy without containing interesting novel insight.

2. APPLICATION TO DISLOCATION WALLS

Figure 3 shows the setting of dislocation walls in $[0, L] \times h\mathbb{T}$, where $L, h > 0$ and \mathbb{T} is the one-dimensional torus. Dislocation walls are vertically periodic arrays of edge dislocations which are a distance h apart. We consider both walls of ‘positive’ edge dislocations and walls of ‘negative’ edge dislocations, where the sign is related to the orientation of the dislocations. While in [DPG15] the negative walls have vertically a phase shift of $\phi = \frac{1}{2}h$, we allow for any phase shift $\phi \in [\frac{1}{4}h, \frac{3}{4}h]$. For any such ϕ , the force between walls of opposite sign is always repelling.

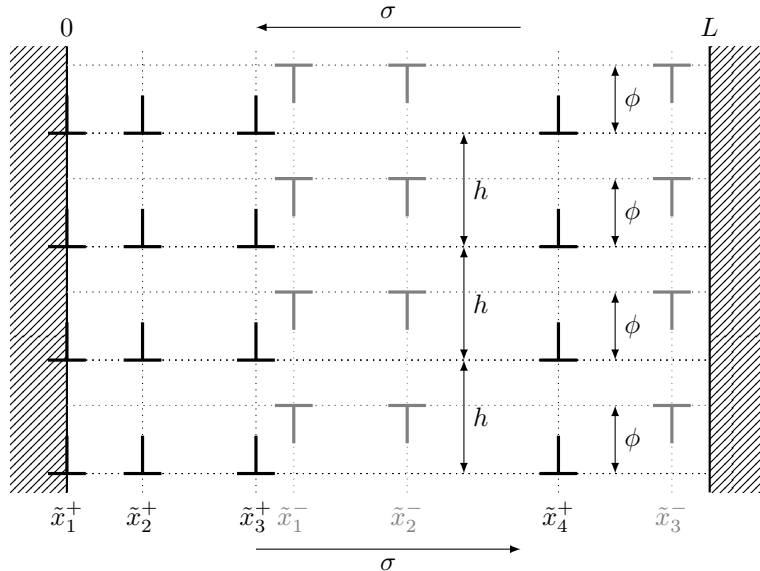


FIGURE 3. Example of $n^+ = 4$ positive dislocation walls and $n^- = 3$ negative dislocation walls. The domain is vertically periodic with period h . Its dimensionless equivalent is illustrated in Figure 1.

Taking the dislocation model of Volterra from 1907, the following energy accounts for all dislocation interactions, including the effect of a constant applied shear stress σ :

$$\begin{aligned} \tilde{E}(\tilde{x}^+, \tilde{x}^-) := & K \sum_{i=1}^{n^+} \sum_{j=1}^{i-1} V\left(\pi \frac{\tilde{x}_i^+ - \tilde{x}_j^+}{h}\right) + K \sum_{i=1}^{n^-} \sum_{j=1}^{i-1} V\left(\pi \frac{\tilde{x}_i^- - \tilde{x}_j^-}{h}\right) \\ & + K \sum_{i=1}^{n^+} \sum_{j=1}^{n^-} W_a\left(\pi \frac{\tilde{x}_i^+ - \tilde{x}_j^-}{h}\right) + \sigma \sum_{i=1}^{n^+} \tilde{x}_i^+ + \sigma \sum_{i=1}^{n^-} (L - \tilde{x}_i^-). \end{aligned}$$

Here, $\tilde{x}^\pm := (\tilde{x}_1^\pm, \dots, \tilde{x}_{n^\pm}^\pm) \in \mathbb{R}^{n^\pm}$, K is a material constant, and the interaction potential V is given by

$$V(r) := r \coth r - \log |2 \sinh r|, \quad r \in \mathbb{R}. \quad (11)$$

Figure 2 illustrates V . This potential is a special case of the more general potential in (12), which was first derived in [HL82, (19-75)] (an alternative derivation can be found in [vM15, Prop. A.2.2]). We note that, in the special case where only one type of dislocation walls is considered (i.e., $n^- = 0$ or $n^+ = 0$), \tilde{E} is the same energy as the one studied in [vMMP14]. The interaction potential W_a describes the interaction between positive and negative walls. It is given by

$$W_a(r) := \frac{1}{2} \log(2(\cosh(2r) + a)) - \frac{r \sinh(2r)}{\cosh(2r) + a}, \quad r \in \mathbb{R}, \quad a \in [-1, 1]. \quad (12)$$

Figure 2 illustrates W_a . The parameter a is related to the phase shift $\phi \in [0, h]$ by $a = -\cos 2\pi \frac{\phi}{h}$. We note that $a \in [0, 1]$ corresponds to a phase shift between $\frac{1}{4}h$ and $\frac{3}{4}h$, and that $W_{-1}(r) = -V(r)$, which is consistent with the fact that dislocations of opposite sign interact with opposite force.

Proposition 2.1 (Properties of W_a). *It holds that*

- (i) $W_a \in \mathcal{S}(\mathbb{R})$ for all $-1 < a \leq 1$;
- (ii) $0 < W_0 \leq W_a < W_b \leq W_1 < V$ on \mathbb{R} for all $0 \leq a < b \leq 1$;
- (iii) $V - W_a$ is strictly convex on $(0, \infty)$ for all $0 \leq a \leq 1$;
- (iv) $\widehat{W}_a > 0$ for all $0 \leq a \leq 1$.

We are interested in the many-particle limit of \tilde{E} . To find a meaningful limit, it is essential to find a proper rescaling of the wall positions \tilde{x}^\pm and of the energy \tilde{E} in terms of the physical parameters K_n , σ_n and h_n . The precise dependence of these parameters on n is a modelling choice, which we choose to keep general. We use the same scaling as in [SPPG14] and [vMMP14]. Setting

$$\alpha_n := \frac{\pi L_n}{h_n}, \quad \gamma_n := L_n \sqrt{\frac{\pi \sigma_n}{n K_n h_n}}$$

as dimensionless parameters¹, and rescaling the particle positions and energy as

$$x_i^\pm := \frac{\tilde{x}_i^\pm}{L_n} \quad \text{and} \quad E_n(x^{n,+}, x^{n,-}) := \frac{\pi L_n}{n^2 K_n h_n} \tilde{E}(L_n x^{n,+}, L_n x^{n,-}),$$

we obtain that rescaled energy E_n is given by (2).

Regarding dislocation dynamics, we rely on the simplest but widely used relation given by Orowan's linear drag law [HB01, (3.3b)]. It states that $v = BF$, where F is the horizontal component of the force acting on the dislocation, v is the horizontal velocity of the dislocation, and B is a constant drag coefficient. By the imposed vertical periodicity in Figure 3, the velocity of a dislocation wall is given by the velocity of each single dislocation in the wall. Hence, by absorbing B in the time variable, we obtain (7).

¹The only difference with [vMMP14] is that we take α_n n times larger

3. NOTATION AND FUNCTIONAL FRAMEWORK

Here we list the symbols and notation which we use in the remainder of this paper:

$a \wedge b, a \vee b$	$\min\{a, b\}, \max\{a, b\}$	
f_{eff}	$f_{\text{eff}}(x) := \sum_{k=1}^{\infty} f(kx)$	
$\ f\ _q$	L^q -norm of f on the domain of f	
$\widehat{f}, \mathcal{F}(f)$	Fourier transform of f ; $\mathcal{F}(f)(\omega) = \widehat{f}(\omega) := \int_{\mathbb{R}} f(x) e^{-2\pi i x \omega} dx$	
$\mu \otimes \nu$	product measure; $(\mu \otimes \nu)(A \times B) = \mu(A)\nu(B)$	
$\mu_n \boxtimes \mu_n$	product measure ‘without the diagonal’	(13)
$\mathbb{1}_A$	$\mathbb{1}_A(x)$ equals 1 if $x \in A$ and 0 if $x \notin A$	
$\boldsymbol{\mu}$	$\boldsymbol{\mu} := (\mu^+, \mu^-) \in M([0, 1])$	
$\mathcal{M}_+([0, 1])$	Space of finite, non-negative Borel measures on $[0, 1]$	
$\mathcal{M}([0, 1]; [0, \infty)^2)$	$[0, \infty)^2$ -valued finite Borel measures on $[0, 1]$	
$M([0, 1])$	Domain of E ; $M([0, 1]) \subset \mathcal{M}([0, 1]; [0, \infty)^2)$	(15)
\mathbb{N}	$\{1, 2, 3, \dots\}$	
$\mathcal{P}([0, 1])$	Space of probability measures; $\mathcal{P}([0, 1]) = \{\mu \in \mathcal{M}_+([0, 1]) : \mu([0, 1]) = 1\}$	
$W(\mu, \nu)$	2-Wasserstein distance between $\mu, \nu \in \mathcal{P}([0, 1])$	[AGS08]
$\mathbf{W}(\boldsymbol{\mu}, \boldsymbol{\nu})$	Modified Wasserstein distance between $\boldsymbol{\mu}, \boldsymbol{\nu} \in M([0, 1])$	(73)

For μ_n^\pm as in (3), we set

$$\mu_n^\pm \boxtimes \mu_n^\pm := \frac{1}{n^2} \sum_{i=1}^{n^\pm} \sum_{\substack{j=1 \\ j \neq i}}^{n^\pm} \delta_{(x_i^\pm, x_j^\pm)} \in \mathcal{M}([0, 1]^2) \quad (13)$$

as the product measure ‘without the diagonal’. We recall from [GPPS13, Lem. 1] and [Bil68, §3.4] that $\mu_n^\pm \rightharpoonup \mu^\pm$ implies

$$\begin{aligned} \mu_n^\pm \boxtimes \mu_n^\pm &\rightharpoonup \mu^\pm \otimes \mu^\pm \quad \text{as } n \rightarrow \infty, \text{ and} \\ \mu_n^+ \otimes \mu_n^- &\rightharpoonup \mu^+ \otimes \mu^- \quad \text{as } n \rightarrow \infty. \end{aligned} \quad (14)$$

The domain of the limit energy E defined in Theorem 1.1 is given by

$$M([0, 1]) := \{\boldsymbol{\mu} := (\mu^+, \mu^-) \in \mathcal{M}_+([0, 1]) \times \mathcal{M}_+([0, 1]) : \mu^+ + \mu^- \in \mathcal{P}([0, 1])\}, \quad (15)$$

In the special case when μ^\pm are *absolutely continuous*, i.e.,

$$\text{there exist } \rho^\pm \in L_+^1(0, 1) \text{ such that } d\mu^\pm(x) = \rho^\pm(x) dx, \quad (16)$$

we denote by $\boldsymbol{\rho} := (\rho^+, \rho^-)$ their density.

We prove Theorem 1.1 separately for each of the three scaling regimes of α_n as outlined in Table 1. We establish the corresponding Γ -convergence result by proving the following two inequalities for all $\boldsymbol{\mu} \in M([0, 1])$:

$$\text{for all } \boldsymbol{\mu}_n \rightharpoonup \boldsymbol{\mu}, \quad \liminf_{n \rightarrow \infty} E_n(\boldsymbol{\mu}_n) \geq E(\boldsymbol{\mu}), \quad (17a)$$

$$\text{there exists } \boldsymbol{\mu}_n \rightharpoonup \boldsymbol{\mu} \text{ such that } \limsup_{n \rightarrow \infty} E_n(\boldsymbol{\mu}_n) \leq E(\boldsymbol{\mu}), \quad (17b)$$

where $\boldsymbol{\mu}_n \rightharpoonup \boldsymbol{\mu}$ if and only if $\mu_n^+ \rightharpoonup \mu^+$ and $\mu_n^- \rightharpoonup \mu^-$. The expression for E depends on the scaling regime of α_n . Any sequence $(\boldsymbol{\mu}_n)$ satisfying (17b) is called a *recovery sequence*.

A basic property of Γ -convergence is that it is stable under *continuously converging* perturbations. A sequence of functionals (G_n) converges continuously to G if

$$\text{for all } \boldsymbol{\mu}_n \rightharpoonup \boldsymbol{\mu}, \quad G_n(\boldsymbol{\mu}_n) \xrightarrow{n \rightarrow \infty} G(\boldsymbol{\mu}). \quad (18)$$

Then, Γ -convergence of E_n to E being stable under continuously converging perturbations means that $(E_n + G_n)$ Γ -converges to $(E + G)$ for all (G_n) converging continuously to G .

4. PROOF OF THEOREM 1.1

We observe from (4) that the last two terms of E_n in the right-hand side of (2) converge continuously (see (18)), and thus it suffices to focus on the first three terms describing the interactions. Therefore, in this section, we set $\gamma_n = \gamma = 0$ without loss of generality.

Throughout this section, we use the following symmetry of E_n between positive and negative particles

$$E_n(x^{n,+}, x^{n,-}) = E_n(\mathbf{1}^{n,-} - x^{n,-}, \mathbf{1}^{n,+} - x^{n,+}), \quad (19)$$

where $\mathbf{1}^{n,\pm} := (1, \dots, 1)^T \in \mathbb{R}^{n^\pm}$. Hence, any statement on positive particles implies a similar statement on the negative particles.

4.1. The case $\alpha_n \rightarrow \alpha > 0$. We note that E_n can be rewritten as

$$E_n(x^{n,+}, x^{n,-}) = E_n^+(x^{n,+}) + E_n^-(x^{n,-}) + \frac{1}{n^2} \sum_{i=1}^{n^+} \sum_{j=1}^{n^-} \alpha_n W(\alpha_n(x_i^+ - x_j^-)), \quad (20)$$

where

$$E_n^\pm : \Omega_n^\pm \rightarrow [0, \infty), \quad E_n^\pm(x^{n,\pm}) := \frac{1}{n^2} \sum_{i=1}^{n^\pm} \sum_{j=1}^{i-1} \alpha_n V(\alpha_n(x_i^\pm - x_j^\pm)),$$

are equivalent to the energy considered in [vMMP14] (except for the argument of E_n^\pm being a vector of size n^\pm instead of n).

Assumption 4.1 (Properties of V and W in case $\alpha_n \rightarrow \alpha > 0$). *V and W satisfy*

- (i) $V = V_{\text{sing}} + V_{\text{reg}}$, where $V_{\text{reg}} \in C(\mathbb{R})$ is even, and $V_{\text{sing}} \in L_{\text{loc}}^1(\mathbb{R})$ is even, non-negative and decreasing on $(0, \infty)$;
- (ii) $W \in C(\mathbb{R})$ is even.

Lemma 4.2 (Γ -convergence of E_n^\pm [GPPS13]). *Let $\gamma_n \rightarrow \gamma \in [0, \infty)$, $\alpha_n \rightarrow \alpha \in (0, \infty)$, and let V satisfy Assumption 4.1. Then E_n^\pm Γ -converges to*

$$\mu^\pm \mapsto \frac{1}{2} \int_0^1 \int_0^1 \alpha V(\alpha(x-y)) d(\mu^\pm \otimes \mu^\pm)(x, y).$$

Moreover, a recovery sequence in (17b) can be constructed for any prescribed n^\pm which satisfies $\frac{1}{n}n^\pm \rightarrow \mu^\pm([0, 1])$ as $n \rightarrow \infty$.

Proof. [GPPS13, Thm. 5] states a similar Γ -convergence result for the setting of the half infinite domain $[0, \infty)$, for a smaller class of potentials V , and for $\sigma_n^\pm := \frac{1}{n}n^\pm = 1$. [vMMP14, Thm. 1.1] extends this result to finite domains, and in [vM15, §3.6] this result is extended to V satisfying Assumption 4.1.

Next we extend to any preset $\sigma_n^\pm \rightarrow \sigma^\pm \in [0, 1]$. If $\sigma^\pm > 0$, then $\sigma_n^\pm > 0$ for all n large enough. Thus, setting $\tilde{\mu}_n^\pm := \mu_n^\pm / \sigma_n^\pm \in \mathcal{P}([0, 1])$ we find from $\mu_n^\pm \rightharpoonup \mu^\pm$ that $\tilde{\mu}_n^\pm \rightharpoonup \mu^\pm / \sigma^\pm =: \tilde{\mu}^\pm$ as $n \rightarrow \infty$. Then, from the unit mass case we infer that

$$\begin{aligned} E_n^\pm(\mu_n^\pm) &= \left(\frac{n^\pm}{n}\right)^2 \frac{1}{(n^\pm)^2} \sum_{i=1}^{n^\pm} \sum_{j=1}^{i-1} \alpha_n V(\alpha_n(x_i^\pm - x_j^\pm)) \\ &= (\sigma_n^\pm)^2 \frac{1}{2} \int_0^1 \int_0^1 \alpha_n V(\alpha_n(x-y)) d(\tilde{\mu}_n^\pm \boxtimes \tilde{\mu}_n^\pm)(x, y) = (\sigma_n^\pm)^2 E_{n^\pm}^\pm(\tilde{\mu}_n^\pm) \end{aligned} \quad (21)$$

Γ -converges to

$$\sigma^2 \frac{1}{2} \int_0^1 \int_0^1 \alpha V(\alpha(x-y)) d(\tilde{\mu}^\pm \otimes \tilde{\mu}^\pm)(x, y) = \frac{1}{2} \int_0^1 \int_0^1 \alpha V(\alpha(x-y)) d(\mu^\pm \otimes \mu^\pm)(x, y).$$

If $\sigma^\pm = 0$, then the Γ -limit equals 0. Indeed, since $V \geq -C$ on $[-\alpha - 1, \alpha + 1]$, the liminf inequality (17a) follows from

$$E_n^\pm(\mu_n^\pm) = \frac{1}{2} \int_0^1 \int_0^1 \alpha V(\alpha(x-y)) d(\mu_n^\pm \otimes \mu_n^\pm)(x, y) \geq -\frac{C}{2} \alpha (\sigma_n^\pm)^2 \xrightarrow{n \rightarrow \infty} 0.$$

For the limsup inequality, we choose μ_n^\pm such that $E_{n^\pm}^\pm(\tilde{\mu}_n^\pm)$ is bounded. Then, by (21), we obtain $E_n^\pm(\mu_n^\pm) = (\sigma_n^\pm)^2 E_{n^\pm}^\pm(\tilde{\mu}_n^\pm) \rightarrow 0$ as $n \rightarrow 0$. \square

Theorem 4.3 (Γ -convergence of E_n in case $\alpha_n \rightarrow \alpha > 0$). *Let $\alpha_n \rightarrow \alpha > 0$, and let V and W satisfy Assumption 4.1. Then E_n Γ -converges to*

$$E(\mu^+, \mu^-) = \frac{1}{2} \iint_{[0,1]^2} \alpha V(\alpha(x-y)) d(\mu^+ \otimes \mu^+ + \mu^- \otimes \mu^-)(x, y) \\ + \iint_{[0,1]^2} \alpha W(\alpha(x-y)) d(\mu^+ \otimes \mu^-)(x, y).$$

Moreover, the recovery sequence in (17b) can be constructed for any prescribed n^\pm which satisfies $\frac{1}{n} n^\pm \rightarrow \mu^\pm([0, 1])$ as $n \rightarrow \infty$.

Proof. In terms of the measures μ_n^\pm , (20) reads

$$E_n(\mu_n^+, \mu_n^-) = E_n^+(\mu_n^+) + E_n^-(\mu_n^-) + \iint_{[0,1]^2} \alpha_n W(\alpha_n(x-y)) d(\mu_n^+ \otimes \mu_n^-)(x, y). \quad (22)$$

Firstly, since $W \in C(\mathbb{R})$ and $|x-y| \leq 1$, the sequence of maps $(x, y) \mapsto \alpha_n W(\alpha_n(x-y))$ converges uniformly on $[0, 1]^2$ to $\alpha W(\alpha(x-y))$. Secondly, for any $\mu_n^\pm \rightharpoonup \mu^\pm$, we have by (14) that $\mu_n^+ \otimes \mu_n^- \rightharpoonup \mu^+ \otimes \mu^-$. Together, these properties imply that the third term in the right-hand side of (22) converges to

$$\iint_{[0,1]^2} \alpha W(\alpha(x-y)) d(\mu^+ \otimes \mu^-)(x, y),$$

and thus it is a continuous perturbation (18) to the other two terms in (22). Γ -convergence of these two terms follows from Lemma 4.2 and the observation that they decouple the dependence of E_n on μ_n^+ and μ_n^- . \square

4.2. The case $1 \ll \alpha_n \ll n$.

Assumption 4.4 (Properties of V and W in case $1 \ll \alpha_n \ll n$). *V and W satisfy*

- (i) $V \in L^1(\mathbb{R})$ is even, and non-increasing on $(0, \infty)$;
- (ii) $W \in L^1(\mathbb{R}) \cap C(\mathbb{R})$ is even, satisfies $\mathcal{F}W \geq 0$, and is non-increasing on $(0, \infty)$;
- (iii) $V - W \not\equiv 0$ can be approximated by $U^\delta \nearrow (V - W)$ pointwise a.e. on \mathbb{R} as $\delta \rightarrow 0$, where $\mathcal{F}U^\delta \geq 0$ and $U^\delta(0) < \infty$ for all $\delta > 0$.

A typical example of a couple (V, W) which satisfies Assumption 4.4 is given by W as in (ii), and $V \in L^1(\mathbb{R})$ even on \mathbb{R} with $V'' \geq W'' \vee 0$ on $(0, \infty)$. Then, a possible choice for U^δ is the convex envelope of

$$x \mapsto \begin{cases} V(x) - W(x) & x > 0, \\ \delta^{-1} & x = 0 \end{cases}$$

with even extension from $x \in [0, \infty)$ to $x \in \mathbb{R}$. Proposition 2.1 implies that V and W_a as in (11) and (12) satisfy Assumption 4.4 for all $a \in [0, 1]$.

We assume non-negativity of the Fourier transform in Assumption 4.4 to rule out the formation of microstructures in $x^{n,\pm}$ which could lower the energy. We sketch the argument on how non-negativity of the Fourier transform prevents such low-energy microstructures, and refer for the details to [GPPS13] and [vM15, §3.6]. We first consider the single particle case $n^- = 0$, in which we set $W = 0$. The approximation from below by U^δ allows us to include the self-interactions by

$$\frac{1}{2} \iint \alpha_n V(\alpha_n(x-y)) d(\mu_n^+ \boxtimes \mu_n^+)(x, y) \geq \frac{1}{2} \iint \alpha_n U^\delta(\alpha_n(x-y)) d(\mu_n^+ \otimes \mu_n^+)(x, y) - \frac{\alpha_n}{2n} U^\delta(0).$$

The non-negativity of $\mathcal{F}U^\delta$ allows us to split the operation ‘convolution with U^δ ’ as applying twice the convolution with u^δ , i.e., $U^\delta = u^\delta * u^\delta$. Setting $U_n^\delta := \alpha_n U^\delta(\alpha_n \cdot)$, we obtain

$$\frac{1}{2} \iint U_n^\delta(x-y) d(\mu_n^+ \otimes \mu_n^+)(x, y) = \frac{1}{2} \int_{\mathbb{R}} (u_n^\delta * \mu_n^+)^2(x) dx.$$

This approximation of E_n from below by the square of the L^2 -norm of $u_n^\delta * \mu_n^+$ is the key for deriving the following Γ -liminf estimate, and the author is unaware of any other technique which leads to the same lower bound.

Lemma 4.5 (Γ -liminf inequality of E_n^\pm [GPPS13, Thm. 7]). *Let $1 \ll \alpha_n \ll n$ and let V satisfy Assumption 4.4.(iii) (with $V = V - W$). Then, for all $\mu_n^\pm \rightharpoonup \mu^\pm$ it holds that*

$$\liminf_{n \rightarrow \infty} \frac{1}{2} \int_0^1 \int_0^1 \alpha_n V(\alpha_n(x-y)) d(\mu_n^\pm \boxtimes \mu_n^\pm)(x, y) \geq \left(\int_0^\infty V \right) \int_0^1 \rho^\pm(x)^2 dx,$$

where the right-hand side is defined as ∞ if μ^\pm is not absolutely continuous (cf. 16).

In the proof of Theorem 1.1, we apply Lemma 4.5 twice; once with $V = V - W$ and once with $V = W$.

In the case of mixed particles, a similar strategy for obtaining a sufficient lower bound results in an additional term given by

$$\frac{1}{2} \int_{\mathbb{R}} (w_n * \mu_n^+)(x) (w_n * \mu_n^-)(x) dx,$$

where $w_n * w_n = W_n := \alpha_n W(\alpha_n \cdot)$. This term is an L^2 -inner-product rather than the square of an L^2 -norm. We bound it from below by using the Cauchy-Schwartz inequality, which leaves us to bound $\|w_n * \mu_n^\pm\|_2^2$ by part of the energy $E_n^\pm(\mu_n^\pm)$. Assumption 4.4.(iii) is chosen to make this estimate work.

For the construction of a recovery sequence (17b), we do not rely on the technique in [GPPS13]. The main reason is that this technique relies on describing the particle positions x_i^+ in terms of the displacement u_n (5), which is not suited in the case of multiple species. Instead, we use the description in terms of μ_n , and construct the recovery sequence similarly as in [MPS14]. We use the assumption that V and W are non-increasing on $(0, \infty)$ to have the monotonicity result that the energy E_n does not decrease whenever we replace the argument of V or W by a number with smaller absolute value.

Theorem 4.6 (Γ -convergence of E_n in case $1 \ll \alpha_n \ll n$). *Let $1 \ll \alpha_n \ll n$, and let V and W satisfy Assumption 4.4. Then E_n Γ -converges to*

$$E(\mu^+, \mu^-) = \left(\int_0^\infty V \right) \int_0^1 (\rho^+(x)^2 + \rho^-(x)^2) dx + \left(\int_0^\infty W \right) \int_0^1 2\rho^+(x)\rho^-(x) dx, \quad (23)$$

where the right-hand side is defined as ∞ if μ^\pm is not absolutely continuous (cf. 16).

Proof. Setting $V_n := \alpha_n V(\alpha_n \cdot)$ and $W_n := \alpha_n W(\alpha_n \cdot)$, we prove the liminf-inequality (17a) by splitting the interaction energies of particles of the same type as

$$\begin{aligned} E_n^\pm(\mu_n^\pm) &= \frac{1}{2} \iint [(V_n - W_n) + W_n](x-y) d(\mu_n^\pm \boxtimes \mu_n^\pm)(x, y) \\ &= \frac{1}{2} \iint [V_n - W_n](x-y) d(\mu_n^\pm \boxtimes \mu_n^\pm)(x, y) \\ &\quad + \frac{1}{2} \iint W_n(x-y) d(\mu_n^\pm \otimes \mu_n^\pm)(x, y) - \frac{n^\pm}{2n^2} W_n(0). \end{aligned}$$

Then, we rewrite

$$\begin{aligned} E_n(\mu_n^+, \mu_n^-) &= \frac{1}{2} \iint [V_n - W_n](x-y) d(\mu_n^+ \boxtimes \mu_n^+)(x, y) \\ &\quad + \frac{1}{2} \iint [V_n - W_n](x-y) d(\mu_n^- \boxtimes \mu_n^-)(x, y) \\ &\quad + \frac{1}{2} \iint W_n(x-y) d((\mu_n^+ + \mu_n^-) \otimes (\mu_n^+ + \mu_n^-))(x, y) - \frac{\alpha_n}{2n} W(0). \end{aligned}$$

Next we take $\liminf_{n \rightarrow \infty}$ on all four terms in the right-hand side separately. The $\liminf_{n \rightarrow \infty}$ of the first three terms are given by Lemma 4.5, and since $\alpha_n \ll n$, the fourth term converges to 0.

We establish the limsup-inequality (17b) by constructing a recovery sequence for μ in a dense subset of $M([0, 1])$, which is similar to one used in [MPS14]. To construct this subset, we divide the domain of the dislocation walls in closed intervals I_k with $k = 1, \dots, K$ as in Figure 4, with size $\varepsilon > 0$ such that the intervals fit ‘nicely’, i.e., $K\varepsilon(1 + \varepsilon) = 1$.

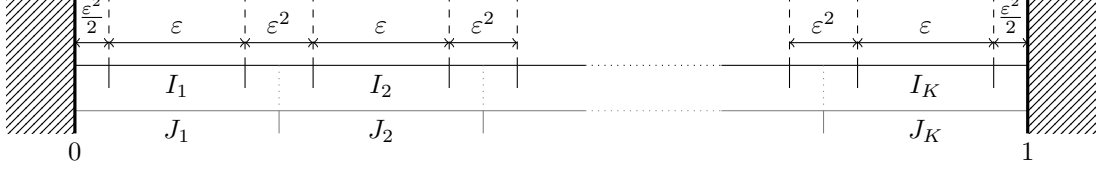


FIGURE 4. Location of the closed intervals I_k of length ε and intervals $J_k \supset I_k$ of length $\varepsilon(1 + \varepsilon)$.

The dense subset consists of all densities ρ^\pm which are piecewise constant on the intervals I_k and 0 elsewhere, viz.

$$\rho^\pm := \sum_{k=1}^K \sigma_k^\pm \mathbb{1}_{I_k}, \quad (24)$$

where the constants $\sigma_k^\pm \geq 0$ satisfy $\varepsilon \sum_{k=1}^K (\sigma_k^+ + \sigma_k^-) = 1$, and $K \in \mathbb{N}$. Since E as in (23) is continuous in $L^2(0, 1; \mathbb{R}^2)$, it is enough to show that this subset is dense in $L^2(0, 1; \mathbb{R}^2) \cap M([0, 1])$ with respect to the L^2 -norm. This is straightforward; it is clearly L^2 -dense in $C([0, 1]; \mathbb{R}^2) \cap M([0, 1])$, whose closure in the L^2 -norm equals $L^2(0, 1; \mathbb{R}^2) \cap M([0, 1])$.

It remains to construct x^n for any ρ^\pm as in (24). For $n \in \mathbb{N}$, we set $\sigma := \int_0^1 \rho$, note that $\sigma^+ + \sigma^- = 1$, and choose $n^\pm \in \mathbb{N} \cup \{0\}$ such that $|n^\pm - n\sigma^\pm| \leq \frac{1}{2}$ and $n^+ + n^- = n$. We build the recovery sequence in the locally equidistant way:

$$\int_0^{x_i^\pm} \rho^\pm(x) dx := \frac{i - \frac{1}{2}}{n}, \quad \text{for } i = 1, \dots, n^\pm.$$

We note that $x_i \in \cup_{k=1}^K I_k$ for all i , define

$$n_k^\pm := \#\{i : x_i^\pm \in I_k\},$$

and relabel the particle positions in I_k as $x_i^{k, \pm}$ for $i = 1, \dots, n_k^\pm$. We note that

$$\varepsilon \sigma_k^\pm \geq \int_{x_1^{k, \pm}}^{x_{n_k^\pm}^{k, \pm}} \rho^\pm(x) dx = \frac{n_k^\pm - 1}{n},$$

and thus $n_k^\pm \leq \varepsilon n \sigma_k^\pm + 1$.

Next we estimate the interaction energy. We start with the interactions between particles of the same type:

$$E_n^\pm(x^{n, \pm}) = \frac{1}{n^2} \sum_{k=1}^K \sum_{i=1}^{n_k^\pm} \left[\sum_{j=1}^{i-1} V_n(x_i^{k, \pm} - x_j^{k, \pm}) + \sum_{j=1}^{N_k} V_n(x_i^{k, \pm} - x_j^\pm) \right], \quad (25)$$

where $N_k := \sum_{\ell=1}^{k-1} n_\ell^\pm$. For the first term in the right-hand side, we use that $x_i^{k, \pm} - x_j^{k, \pm} = (i - j)/(n\sigma_k^\pm)$, and estimate

$$\begin{aligned} \frac{1}{n^2} \sum_{k=1}^K \sum_{i=1}^{n_k^\pm} \sum_{j=1}^{i-1} V_n(x_i^{k, \pm} - x_j^{k, \pm}) &\leq \frac{1}{n^2} \sum_{k=1}^K \sum_{i=1}^{n_k^\pm} \sum_{j=1}^{\infty} V_n\left(\frac{j}{n\sigma_k^\pm}\right) \\ &= \frac{1}{n^2} \sum_{k=1}^K n_k^\pm n \sigma_k^\pm \sum_{j=1}^{\infty} \frac{\alpha_n}{n \sigma_k^\pm} V\left(\frac{\alpha_n j}{n \sigma_k^\pm}\right) \leq \frac{1}{n} \sum_{k=1}^K (\varepsilon n \sigma_k^\pm + 1) \sigma_k^\pm \left(\int_0^\infty V \right). \end{aligned}$$

Expanding the parenthesis, we obtain from $\sum_{k=1}^K \sigma_k^\pm = \sigma^\pm/\varepsilon$ that the term related to ‘+1’ is of the order of $\frac{1}{n}$, which vanishes in the limit $n \rightarrow \infty$. For the other term, we observe that

$$\left(\int_0^\infty V \right) \varepsilon \sum_{k=1}^K (\sigma_k^\pm)^2 = \left(\int_0^\infty V \right) \int_0^1 (\rho^\pm)^2,$$

which is independent of n . In conclusion, we obtain for the first term in (25) that

$$\limsup_{n \rightarrow \infty} \frac{1}{n^2} \sum_{k=1}^K \sum_{i=1}^{n_k^\pm} \sum_{j=1}^{i-1} V_n(x_i^{k,\pm} - x_j^{k,\pm}) \leq \left(\int_0^\infty V \right) \int_0^1 (\rho^\pm)^2.$$

For the second term in the right-hand side of (25), we estimate

$$x_i^{k,\pm} - x_j^\pm = (x_i^{k,\pm} - x_{N_k}^\pm) + (x_{N_k}^\pm - x_j^\pm) \geq \varepsilon^2 + \frac{N_k - j}{n \|\rho^\pm\|_\infty}.$$

Since V is non-increasing on $(0, \infty)$, we estimate

$$\begin{aligned} \frac{1}{n^2} \sum_{k=1}^K \sum_{i=1}^{n_k^\pm} \sum_{j=1}^{N_k} V_n(x_i^{k,\pm} - x_j^\pm) &\leq \frac{1}{n^2} \sum_{k=1}^K \sum_{i=1}^{n_k^\pm} \sum_{j=0}^{N_k-1} V_n\left(\varepsilon^2 + \frac{j}{n \|\rho^\pm\|_\infty}\right) \\ &\leq \frac{1}{n^2} n^\pm \sum_{j=0}^\infty n \|\rho^\pm\|_\infty \frac{\alpha_n}{n \|\rho^\pm\|_\infty} V\left(\alpha_n \varepsilon^2 + \frac{\alpha_n j}{n \|\rho^\pm\|_\infty}\right) \leq \frac{\alpha_n}{n} V(\alpha_n \varepsilon^2) + \|\rho^\pm\|_\infty \left(\int_{\alpha_n \varepsilon^2}^\infty V \right). \end{aligned}$$

From $1 \ll \alpha_n \ll n$ we observe that the right-hand side converges to 0 as $n \rightarrow \infty$. Reflecting back on (25), we obtain

$$\limsup_{n \rightarrow \infty} E_n^\pm(x^{n,\pm}) \leq \left(\int_0^\infty V \right) \int_0^1 (\rho^\pm)^2.$$

It remains to estimate the interactions between particles of opposite type:

$$\frac{1}{n^2} \sum_{k=1}^K \sum_{i=1}^{n_k^+} \left[\sum_{j=1}^{n_k^-} W_n(x_i^{k,+} - x_j^{k,-}) + \sum_{\substack{\ell=1 \\ \ell \neq k}}^K \sum_{j=1}^{n_\ell^-} W_n(x_i^{k,+} - x_j^{\ell,-}) \right]. \quad (26)$$

The second term accounts for all interactions between particles that are contained in different intervals I_k . Analogously to the case of particles of the same type, we can show that this term vanishes in the limit $n \rightarrow \infty$. We skip the details.

Regarding the first term in the right-hand side of (26), we first estimate $|x_i^{k,+} - x_j^{k,-}|$ from below. For fixed $1 \leq k \leq K$ and $1 \leq i \leq n_k^+$, we set

$$J := \max\{j : x_j^{k,-} \leq x_i^{k,+}\} \vee 0.$$

Together with $x_{j+\ell}^{k,-} - x_j^{k,-} = \ell/(n\sigma_k^-)$, we obtain

$$|x_i^{k,+} - x_j^{k,-}| \leq \frac{1}{n\sigma_k^-} \begin{cases} J - j & \text{if } j \leq J, \\ j - (J + 1) & \text{if } j \geq J + 1. \end{cases}$$

Then, since W is non-increasing on $(0, \infty)$, we obtain, similarly to the case of particles of the same type,

$$\begin{aligned} \frac{1}{n^2} \sum_{k=1}^K \sum_{i=1}^{n_k^+} \sum_{j=1}^{n_k^-} W_n(x_i^{k,+} - x_j^{k,-}) &\leq \frac{1}{n^2} \sum_{k=1}^K 2n_k^+ \sum_{j=0}^\infty W_n\left(\frac{j}{n\sigma_k^-}\right) \\ &= \frac{2}{n^2} \sum_{k=1}^K n_k^+ \left[W_n(0) + \sum_{j=1}^\infty n\sigma_k^- \frac{\alpha_n}{n\sigma_k^-} W\left(\frac{\alpha_n j}{n\sigma_k^-}\right) \right] \leq \frac{2}{n} \sum_{k=1}^K (\varepsilon n\sigma_k^+ + 1) \left(\frac{\alpha_n}{n} W(0) + \sigma_k^- \int_0^\infty W \right) \\ &= 2\varepsilon \sum_{k=1}^K \sigma_k^+ \sigma_k^- \left(\int_0^\infty W \right) + \mathcal{O}\left(\frac{\alpha_n}{n}\right) = \left(\int_0^\infty W \right) \int_0^1 2\rho^+ \rho^- + \mathcal{O}\left(\frac{\alpha_n}{n}\right). \end{aligned}$$

Hence, the $\limsup_{n \rightarrow \infty}$ of (26) is bounded from above by $(\int_0^\infty W) \int_0^1 2\rho^+ \rho^-$, which completes the proof of (17b). \square

4.3. The case $\frac{1}{n}\alpha_n \rightarrow \alpha > 0$. We use the description of $x^{n,\pm}$ in terms of x^n and b^n as introduced above (7). Defining

$$V_{ij} := \begin{cases} V & \text{if } b_i b_j = 1, \\ W & \text{if } b_i b_j = -1, \end{cases}$$

the expression for the energy E_n in (2) can be written compactly as

$$E_n(x^n) = \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^{i-1} \alpha_n V_{ij} (\alpha_n (x_i - x_j)).$$

We switch between these different descriptions whenever convenient.

Assumption 4.7 (Properties of V and W in case $\alpha_n/n \rightarrow \alpha > 0$). *V and W satisfy*

- (i) $V : \mathbb{R} \setminus \{0\} \rightarrow [0, \infty)$ is even, lower semi-continuous on \mathbb{R} with $V(0) = \infty$, non-increasing on $(0, \infty)$, and satisfies $\int_1^\infty V < \infty$;
- (ii) $W \in L^\infty(\mathbb{R}) \cap L^1(\mathbb{R})$ is even, and non-increasing on $(0, \infty)$;
- (iii) $V \geq W$.

Remark 4.8 (Consequences of Assumption 4.7). *The monotonicity and integrability of W implies that $W \geq 0$. We further note that $xV_{\text{eff}}(x)$ and $xW_{\text{eff}}(x)$ are Riemann lower-sums for $\int_0^\infty V$ and $\int_0^\infty W$ respectively. Hence,*

$$V_{\text{eff}}, W_{\text{eff}} \in L^\infty(\delta, \infty) \quad \text{for any } \delta > 0.$$

Furthermore, by the monotonicity of V , $V|_{(0, \infty)}$ has a pseudo-inverse $V^{-1} : (0, \infty) \rightarrow (0, \infty)$, which has finite integral on $(0, M)$ for any $M > 0$. We obtain

$$xV_{\text{eff}}(x) \leq xV(x) + \int_x^\infty V = \int_0^{V(x)} V^{-1} \xrightarrow{x \rightarrow \infty} 0. \quad (27)$$

In a similar spirit as in [BG04], the Γ -limit of the interactions is determined implicitly through a cell energy density $\psi : [0, \infty)^2 \rightarrow [0, \infty)$. We define ψ as

$$\psi(\sigma^+, \sigma^-) := \lim_{m \rightarrow \infty} \psi_m(\sigma^+, \sigma^-), \quad (28a)$$

$$\begin{aligned} \psi_m(\sigma^+, \sigma^-) &:= 0 \vee \min \left\{ \frac{1}{m} \sum_{i=1}^{\tilde{n}} \sum_{j=1}^{i-1} \alpha V_{ij} (\alpha m [y_i - y_j]) : \tilde{n} := \tilde{n}^+ + \tilde{n}^-, \tilde{n}^\pm := \lfloor \sigma^\pm m \rfloor \right. \\ &\quad \left. 0 \leq y_1^+ \leq \dots \leq y_{\tilde{n}^+}^+ \leq 1, 0 \leq y_1^- \leq \dots \leq y_{\tilde{n}^-}^- \leq 1 \right\}, \end{aligned} \quad (28b)$$

where m is allowed to be any positive real. Lemma 4.10 guarantees that the limit in (28a) exists, and provides further properties of ψ_m and ψ that are essential for our proof of Theorem 1.1. The proof of Lemma 4.10 relies on the Γ -liminf inequality of [GPPS13, Thm. 8] for particles of the same type with convex interaction potential:

Lemma 4.9 (Liminf inequality of E_n^\pm [GPPS13, Thm. 8]). *Let $\frac{1}{n}\alpha_n \rightarrow 1$ and let $V : \mathbb{R} \setminus \{0\} \rightarrow [0, \infty)$ be even on \mathbb{R} , convex on $(0, \infty)$, $\int_1^\infty V < \infty$ and $V(x) \rightarrow \infty$ if $x \rightarrow 0$. Then, for all $\mu_n^\pm \rightharpoonup \mu^\pm$ it holds that*

$$\liminf_{n \rightarrow \infty} E_n^\pm(\mu_n^\pm) \geq \int_0^1 V_{\text{eff}}\left(\frac{1}{\rho^\pm(x)}\right) \rho^\pm(x) dx,$$

where the right-hand side is defined as ∞ if μ^\pm is not absolutely continuous (cf. (16)).

While [GPPS13] focuses on μ^\pm with mass 1, a simple scaling argument as in the proof of Lemma 4.2 implies that Lemma 4.9 also holds for any measure $\mu^\pm \in \mathcal{M}_+([0, 1])$ and any approximating sequence μ_n^\pm with possibly different mass than μ^\pm .

In Lemma 4.9 and Lemma 4.10 we set $\alpha = 1$, for the simple reason that Assumption 4.7 is invariant under the rescaling $V_\alpha = \alpha V(\alpha \cdot)$ and $W_\alpha = \alpha W(\alpha \cdot)$.

Lemma 4.10 (Properties of ψ_m and ψ). *Set $\alpha = 1$. For any $\sigma = (\sigma^+, \sigma^-) \in [0, \infty)^2$, $\psi_\infty(\sigma) := \psi(\sigma)$ defined by (28a) is well-defined. Moreover, for any $m \in [0, \infty]$*

- (i) $\psi_m(\sigma^+, \sigma^-) = \psi_m(\sigma^-, \sigma^+)$;
- (ii) $\sigma \mapsto \psi_m(\sigma, \sigma^-)$ is non-decreasing;
- (iii) $\psi_m(\sigma) \leq \psi_m(\sigma^+ + \sigma^-, 0)$;
- (iv) $\psi_m(\sigma) \geq \psi_m(\sigma^+, 0) + \psi_m(0, \sigma^-)$;
- (v) $\sigma V_{\text{eff}}(1/\sigma) \geq \psi(\sigma, 0) \geq c(\sigma^2 - C)$ for some $C, c > 0$ independent of σ ;
- (vi) $\psi \in C([0, \infty)^2)$;
- (vii) ψ_m converges continuously to ψ as $m \rightarrow \infty$, i.e., for all $\sigma^\pm \geq 0$ and all $0 \leq \sigma_m^\pm \rightarrow \sigma^\pm$ it holds that $\psi_m(\sigma_m^+, \sigma_m^-) \rightarrow \psi(\sigma^+, \sigma^-)$.

Proof. We note that (i)–(iv) are basic observations, relying only on $0 \leq W \leq V$ being even functions.

As a preliminary step to proving that the limit in (28a) exists, we show that

$$\psi_m(\sigma, 0) \leq \sigma V_{\text{eff}}(1/\sigma) \quad \text{for all } m \geq \frac{1}{\sigma}, \quad (29)$$

$$\liminf_{m \rightarrow \infty} \psi_m(\sigma, 0) \geq c(\sigma^2 - C) \quad \text{for some } C, c > 0 \text{ independent of } \sigma, \quad (30)$$

which together imply (v). We establish (29) by bounding from above the minimisation problem in (28b), given by $\psi_m(\sigma, 0)$, by the equidistant configuration $z_i := (i-1)/(\tilde{n}-1)$, where $\tilde{n} := \lfloor \sigma m \rfloor$. We obtain

$$\psi_m(\sigma, 0) \leq \frac{1}{m} \sum_{k=1}^{\tilde{n}} \sum_{j=1}^{k-1} V(m(z_{k+j} - z_j)) \leq \frac{\tilde{n}-1}{m} \sum_{k=1}^{\tilde{n}} V\left(\frac{m}{\tilde{n}-1}k\right) \leq \frac{\tilde{n}-1}{m} V_{\text{eff}}\left(\frac{m}{\tilde{n}-1}\right).$$

Since V is non-increasing on $(0, \infty)$, V_{eff} is also non-increasing on $(0, \infty)$, and thus (29) follows by using $(\tilde{n}-1)/m < \sigma$. To prove (30), we set V^{**} as the even extension of the convex envelope of V on $(0, \infty)$. Applying Lemma 4.9 with V^{**} , we find

$$\liminf_{m \rightarrow \infty} \psi_m(\sigma, 0) \geq \inf \left\{ \int_0^1 (V^{**})_{\text{eff}}\left(\frac{1}{\rho(x)}\right) \rho(x) dx : \rho \in L_+^1(0, 1) \text{ with } \int_0^1 \rho = \sigma \right\}.$$

Since V^{**} is convex, $r \mapsto r(V^{**})_{\text{eff}}(\frac{1}{r})$ is convex, and thus it follows from Jensen's Inequality that

$$\liminf_{m \rightarrow \infty} \psi_m(\sigma, 0) \geq \sigma(V^{**})_{\text{eff}}\left(\frac{1}{\sigma}\right).$$

Using that V is non-increasing, we find $\int_0^\infty V^{**} \geq \frac{1}{2} \int_0^\infty V > 0$. Since $\frac{1}{\sigma}(V^{**})_{\text{eff}}(\frac{1}{\sigma})$ is a Riemann lower-sum of V^{**} , it holds that $\lim_{\sigma \rightarrow \infty} \frac{1}{\sigma}(V^{**})_{\text{eff}}(\frac{1}{\sigma}) \geq \frac{1}{2} \int_0^\infty V \in (0, \infty]$, and thus there exists a $c > 0$ such that

$$\sigma(V^{**})_{\text{eff}}\left(\frac{1}{\sigma}\right) \geq c\sigma^2 \quad \text{for all } \sigma \text{ large enough.} \quad (31)$$

We conclude (30).

The remainder of the proof of Lemma 4.10 concerns (vii), which we prove in four steps. Step 1 treats the easiest case where $\sigma = \mathbf{0}$. Steps 2 and 3 establish a continuity estimate on ψ_m , uniform in m (see (32) and (47)). In Step 4 we prove pointwise convergence of ψ_m to ψ as $m \rightarrow \infty$. Steps 1–4 together imply (vii), and hence (i)–(iv) also hold for $m = \infty$. (vi) is a corollary of (vii), because (vii) implies that both ψ_m and $-\psi_m$ Γ -converge to ψ , from which we infer that both ψ and $-\psi$ are lower semi-continuous.

Step 1: (vii) for $\sigma = \mathbf{0}$. Let $\sigma_m \rightarrow \mathbf{0}$ as $m \rightarrow \infty$, and let $\varepsilon > 0$ be arbitrary. We set $\sigma_m = \sigma_m^+ + \sigma_m^-$, and consider m large enough such that $\sigma_m < \varepsilon$. Then (ii), (iii) and (29) imply that

$$\limsup_{m \rightarrow \infty} \psi_m(\sigma_m) \leq \limsup_{m \rightarrow \infty} \psi_m(\sigma_m, 0) \leq \limsup_{m \rightarrow \infty} \psi_m(\varepsilon, 0) \leq \varepsilon V_{\text{eff}}\left(\frac{1}{\varepsilon}\right)$$

for m large enough. We conclude (vii) in case $\sigma = \mathbf{0}$ from the arbitrariness of $\varepsilon > 0$ and (27).

Step 2: continuity estimate for ψ_m at $\sigma^\pm > 0$. In this step we prove the following estimate:

$$\forall \sigma^\pm > 0 \exists C > 0 \forall \delta > 0 \exists M > 0 \forall m > M : \psi_m((1+\delta)\sigma) - \psi_m((1-\delta)\sigma) \leq C\delta. \quad (32)$$

We fix some notation by writing out (28b) in detail:

$$\psi_m((1-\delta)\sigma) = \min \left\{ \frac{1}{m} \sum_{i>j}^{\tilde{n}} V_{ij}(m[y_i - y_j]) : \tilde{n} := \tilde{n}^+ + \tilde{n}^-, \tilde{n}^\pm := \lfloor \sigma^\pm(1-\delta)m \rfloor \right. \\ \left. 0 \leq y_1^+ \leq \dots \leq y_{\tilde{n}^+}^+ \leq 1, 0 \leq y_1^- \leq \dots \leq y_{\tilde{n}^-}^- \leq 1 \right\} \quad (33)$$

$$\psi_m((1+\delta)\sigma) = \min \left\{ \frac{1}{m} \sum_{i>j}^{\tilde{n}_\delta} V_{ij}(m[z_i - z_j]) : \tilde{n}_\delta := \tilde{n}_\delta^+ + \tilde{n}_\delta^-, \tilde{n}_\delta^\pm := \lfloor \sigma^\pm(1+\delta)m \rfloor \right. \\ \left. 0 \leq z_1^+ \leq \dots \leq z_{\tilde{n}_\delta^+}^+ \leq 1, 0 \leq z_1^- \leq \dots \leq z_{\tilde{n}_\delta^-}^- \leq 1 \right\}. \quad (34)$$

Since $\sigma^\pm > 0$, it holds that $\tilde{n}^\pm \rightarrow \infty$ as $m \rightarrow \infty$, and thus for all m large enough we can assume \tilde{n}^\pm to be large enough in the argument below. We also assume $\delta > 0$ to be small enough, independent of m . We fix such m , let y be a minimiser of (33) satisfying $y_1 \leq \dots \leq y_{\tilde{n}}$, and set

$$d_i^\pm := y_{i+1}^\pm - y_i^\pm, \quad c_i^\pm := \frac{1}{2}(y_{i+1}^\pm + y_i^\pm), \quad I^\pm(i) := [y_i^\pm, y_{i+1}^\pm] \quad \text{for all } 1 \leq i \leq \tilde{n}^\pm - 1. \quad (35)$$

We construct an admissible vector $z \in \mathbb{R}^{\tilde{n}_\delta}$ for the minimisation problem in (34) by

$$z_i := \begin{cases} y_i, & 1 \leq i \leq \tilde{n}, \\ c_{\ell_i}, & \tilde{n} + 1 \leq i \leq \tilde{n}_\delta, \end{cases} \quad (36)$$

where $1 \leq \ell_i \leq \tilde{n} - 1$ are carefully chosen indices to find sufficient estimates for the remainder terms Σ_1 and Σ_2 in the following estimate

$$\psi_m((1+\delta)\sigma) \leq \frac{1}{m} \sum_{i>j}^{\tilde{n}_\delta} V_{ij}(m[z_i - z_j]) \\ = \underbrace{\frac{1}{m} \sum_{i>j}^{\tilde{n}} V_{ij}(m[y_i - y_j])}_{\psi_m((1-\delta)\sigma)} + \underbrace{\frac{1}{m} \sum_{i=\tilde{n}+1}^{\tilde{n}_\delta} \sum_{j=\tilde{n}+1}^{i-1} V_{ij}(m[c_{\ell_i} - c_{\ell_j}])}_{\Sigma_1} + \underbrace{\frac{1}{m} \sum_{i=1}^{\tilde{n}} \sum_{j=\tilde{n}+1}^{\tilde{n}_\delta} V_{ij}(m[y_i - c_{\ell_j}])}_{\Sigma_2}. \quad (37)$$

Next we construct the indices ℓ_i such that $\Sigma_1 + \Sigma_2 < C\delta$. To this aim, we put three conditions on ℓ_i . For convenience, we introduce the indices ℓ_i^\pm by the same change of variables which transforms y, b into y^+, y^- . We also introduce the index shift $\kappa_i \geq 1$, which characterises $y_{i+\kappa_i}$ as the next particle with the same sign as y_i .

The first condition on ℓ_i^\pm ensures $d_{\ell_i^\pm}^\pm$ to be large enough. Let s be a permutation such that the interdistances d_i^\pm satisfy $d_{s(1)}^\pm \leq \dots \leq d_{s(\tilde{n}^\pm-1)}^\pm$. We set

$$\tilde{n}_4^\pm := \lfloor \frac{1}{4}(\tilde{n}^\pm - 1) \rfloor, \quad d_*^\pm := d_{s(\tilde{n}_4^\pm)}^\pm, \quad (38)$$

and estimate from below

$$\psi_m((1-\delta)\sigma) \geq \frac{1}{m} \sum_{i=1}^{\tilde{n}_4^+} V(md_{s(i)}^+) \geq \frac{\tilde{n}^+ - 4}{4m} V(md_{s(\tilde{n}_4^+)}^+) \\ = \frac{\lfloor \sigma^+(1-\delta)m \rfloor - 4}{4m} V(md_*^+) \geq \frac{\sigma^+}{5} V(md_*^+) \quad (39)$$

and from above (relying on (ii), (iii) and (29))

$$\psi_m((1-\delta)\sigma) \leq \psi_m(\sigma) \leq \psi_m(\sigma, 0) \leq \sigma V_{\text{eff}}(\frac{1}{\sigma}), \quad (40)$$

where $\sigma = \sigma^+ + \sigma^-$. We obtain that $V(md_*^+) \leq \frac{5\sigma}{\sigma^+} V_{\text{eff}}(\frac{1}{\sigma})$, and thus $d_*^+ \geq \frac{c}{m}$ for some constant $c > 0$ which is independent of δ and m . Since $d_{s(i)}^+$ is ordered in i , we finally obtain

$$d_\ell^+ \geq d_*^+ \geq \frac{c}{m} \quad \text{for all } \ell \in J_1^+ := \{s^{-1}(i) : \tilde{n}_4^+ \leq i \leq \tilde{n}^+ - 1\}. \quad (41)$$

An analogous argument for the negative particles yields

$$d_\ell^- \geq d_*^- \geq \frac{c}{m} \quad \text{for all } \ell \in J_1^- := \{s^{-1}(i) : \tilde{n}_4^- \leq i \leq \tilde{n}^- - 1\} \quad (42)$$

for some (possibly different) permutation s and constant $c > 0$ which is independent of δ and m .

The second condition on the indices ℓ_i^\pm is that the following quantity, which is part of Σ_2 , is bounded uniformly in i , δ and m :

$$\sum_{j=1}^{\ell_i-1} V_{\ell_i j}(m[y_{\ell_i} - y_j]) + \sum_{j=\ell_i+\kappa_{\ell_i}+1}^{\tilde{n}} V_{(\ell_i+\kappa_{\ell_i})j}(m[y_{\ell_i+\kappa_{\ell_i}} - y_j]).$$

We establish the related index sets J_2^\pm by a similar argument to the one leading to J_1^\pm . The main difference is the following bound from below, which follows simply by neglecting several interactions between particles:

$$\psi_m((1-\delta)\sigma) \geq \frac{1}{2m} \sum_{i=1}^{\tilde{n}} \left[\sum_{j=1}^{i-1} V_{ij}(m[y_i - y_j]) + \sum_{j=i+\kappa_i+1}^{\tilde{n}} V_{(i+\kappa_i)j}(m[y_{i+\kappa_i} - y_j]) \right].$$

Then, by introducing permutations s_\pm we can order the summands from high to low values (for the positive and negative particles separately), and estimate the highest $\frac{1}{4}$ -fraction of them by the constant given by the right-hand side of (40) to conclude that

$$\sum_{j=1}^{\ell-1} V_{\ell j}(m[y_\ell - y_j]) + \sum_{j=\ell+\kappa_\ell+1}^{\tilde{n}} V_{(\ell+\kappa_\ell)j}(m[y_{\ell+\kappa_\ell} - y_j]) \leq C$$

for all $\ell \in J_2^\pm := \{s_\pm^{-1}(i) : \tilde{n}_4^\pm \leq i \leq \tilde{n}^\pm\} \quad (43)$

for some constant $C > 0$ which is independent of δ and m .

The third condition on the indices ℓ_i^\pm is that the interval $I^\pm(\ell_i^\pm)$ (see (35)) does not contain too many particles of the opposite sign. Let $N^-(i)$ be the number of negative particles in $I^+(i)$ for $1 \leq i \leq \tilde{n}^+ - 1$, and s_+ be the permutation for which $N^-(s_+(1)) \geq \dots \geq N^-(s_+(\tilde{n}^+ - 1))$. Then,

$$2\tilde{n}^- \geq \sum_{i=1}^{\tilde{n}^+-1} N^-(i) \geq \tilde{n}_4^+ N^-(s_+(\tilde{n}_4^+)),$$

where the factor 2 covers all negative particles located at any of the endpoint of $I^+(i)$, which are counted twice in the sum above. It follows that $N^-(s_+(\tilde{n}_4^+)) \leq K^-$ for some $K^- \in \mathbb{N}$ independent of δ and m . An analogous argument for the positive particles yields $N^+(s_-(\tilde{n}_4^-)) \leq K^+$ for some $K^+ \in \mathbb{N}$. We conclude that

$$N^\mp(\ell) \leq K \quad \text{for all } \ell \in J_3^\pm := \{s_\pm^{-1}(i) : \tilde{n}_4^\pm \leq i \leq \tilde{n}^\pm\} \quad (44)$$

for some constant $K \in \mathbb{N}$ which is independent of δ and m .

We finally construct the set of indices

$$J^\pm := J_1^\pm \cap J_2^\pm \cap J_3^\pm.$$

Since J_1^\pm , J_2^\pm and J_3^\pm contain $\lfloor \frac{3}{4}\tilde{n}^\pm \rfloor$ or more indices, J^\pm contains at least $\lfloor \tilde{n}^\pm/5 \rfloor$ indices, which is enough to choose all the centre points c_{ℓ_i} in (36) differently from each other. Moreover, we use the freedom in this choice to take ℓ_i increasing in i . As a consequence of (41) and (42), we obtain

$$\min\{|c_k^\pm - c_\ell^\pm| : k, \ell \in J^\pm, k \neq \ell\} \geq \frac{c}{m}. \quad (45)$$

Together with the related properties (41)–(45), we estimate the sums Σ_1 and Σ_2 defined in (37). We expand

$$\begin{aligned} \Sigma_1 = \frac{1}{m} \sum_{k=1}^{\tilde{n}_\delta^+ - \tilde{n}^+ - 1} \sum_{j=\tilde{n}^+ + 1}^{\tilde{n}_\delta^+ - k} V\left(m\left[c_{\ell_{k+j}}^+ - c_{\ell_j}^+\right]\right) &+ \frac{1}{m} \sum_{k=1}^{\tilde{n}_\delta^- - \tilde{n}^- - 1} \sum_{j=\tilde{n}^- + 1}^{\tilde{n}_\delta^- - k} V\left(m\left[c_{\ell_{k+j}}^- - c_{\ell_j}^-\right]\right) \\ &+ \frac{1}{m} \sum_{i=\tilde{n}^+ + 1}^{\tilde{n}_\delta^+} \sum_{j=\tilde{n}^- + 1}^{\tilde{n}_\delta^-} W\left(m\left[c_{\ell_i}^+ - c_{\ell_j}^-\right]\right). \end{aligned} \quad (46)$$

Using (45) and V being decreasing on $(0, \infty)$, we estimate the first sum in the right-hand side by

$$\frac{1}{m} \sum_{k=1}^{\tilde{n}_\delta^+ - \tilde{n}^+ - 1} \sum_{j=\tilde{n}^+ + 1}^{\tilde{n}_\delta^+ - k} V\left(m\left[c_{\ell_{k+j}}^+ - c_{\ell_j}^+\right]\right) \leq \frac{1}{m} \sum_{k=1}^{\infty} \sum_{j=\tilde{n}^+ + 1}^{\tilde{n}_\delta^+} V\left(m\left[k \frac{c}{m}\right]\right) = \frac{\tilde{n}_\delta^+ - \tilde{n}^+}{m} V_{\text{eff}}(c) \leq C\delta.$$

The same argument for the negative particles yields the same estimate. We estimate the third sum in the right-hand side of (46) by

$$\begin{aligned} \frac{1}{m} \sum_{i=\tilde{n}^+ + 1}^{\tilde{n}_\delta^+} \sum_{j=\tilde{n}^- + 1}^{\tilde{n}_\delta^-} W\left(m\left[c_{\ell_i}^+ - c_{\ell_j}^-\right]\right) &\leq \frac{1}{m} \sum_{i=\tilde{n}^+ + 1}^{\tilde{n}_\delta^+} \sum_{k=0}^{\infty} 2W\left(m\left[k \frac{c}{m}\right]\right) \\ &= 2 \frac{\tilde{n}_\delta^+ - \tilde{n}^+}{m} (W(0) + W_{\text{eff}}(c)) \leq C\delta, \end{aligned}$$

and conclude that $\Sigma_1 < C\delta$ for a δ - and m -independent constant C .

To estimate Σ_2 , we recall that $z_j^\pm = c_{\ell_j^\pm}^\pm$ is the midpoint of the interval $I^\pm(\ell_j^\pm)$, and split the interactions of y_i with z_j for $y_i \notin I^\pm(\ell_j^\pm)$ and $y_i \in I^\pm(\ell_j^\pm)$. Then, we use (43) to estimate the interactions with $y_i \notin I^\pm(\ell_j^\pm)$, and (44) for those with $y_i \in I^\pm(\ell_j^\pm)$. This yields

$$\begin{aligned} \Sigma_2 &= \frac{1}{m} \sum_{j=\tilde{n}+1}^{\tilde{n}_\delta} \left[\sum_{i: y_i \notin I^\pm(\ell_j^\pm)} V_{i\ell_j}(m[y_i - c_{\ell_j}]) + \sum_{i: y_i \in I^\pm(\ell_j^\pm)} V_{i\ell_j}(m[y_i - c_{\ell_j}]) \right] \\ &\leq \frac{1}{m} \sum_{j=\tilde{n}+1}^{\tilde{n}_\delta} \left[\sum_{i=1}^{\ell_j-1} V_{i\ell_j}(m[y_i - y_{\ell_j}]) + \sum_{i=\ell_i+\kappa_{\ell_i}+1}^{\tilde{n}} V_{i(\ell_i+\kappa_{\ell_i})}(m[y_i - y_{\ell_i+\kappa_{\ell_i}}]) \right. \\ &\quad \left. + \sum_{i: y_i \in I^\pm(\ell_j^\pm)} V_{i\ell_j}(m[y_i - c_{\ell_j}]) \right] \\ &\leq \frac{1}{m} \sum_{j=\tilde{n}+1}^{\tilde{n}_\delta} [C + V(m[c_{\ell_j} - y_{\ell_j}]) + V(m[c_{\ell_j} - y_{\ell_i+\kappa_{\ell_i}}]) + KW(0)] \\ &\leq \frac{\tilde{n}_\delta - \tilde{n}}{m} [C + 2V(m[\frac{c}{2m}])] \leq C\delta. \end{aligned}$$

This concludes the proof for $\Sigma_1 + \Sigma_2 \leq C\delta$, which by (37) implies (32).

Step 3: continuity estimate for ψ_m at $\sigma^+ \wedge \sigma^- = 0$. We establish a similar estimate as (32) in the case when $\sigma^+ \wedge \sigma^- = 0$. By (i) it is enough to prove continuity at the σ^+ -axis, and by Step 1 we can further assume $\sigma := \sigma^+ > 0$. This motivates us to prove

$$\forall \sigma > 0 \exists C > 0 \forall \delta > 0 \exists M > 0 \forall m > M : \psi_m((1+\delta)\sigma, \delta\sigma) - \psi_m((1-\delta)\sigma, 0) \leq C\delta. \quad (47)$$

Since (iii) implies that

$$\psi_m((1+\delta)\sigma, \delta\sigma) - \psi_m((1-\delta)\sigma, 0) \leq \psi_m((1+2\delta)\sigma, 0) - \psi_m((1-\delta)\sigma, 0),$$

the argument in Step 2 (simplified to $n^- = 0$) yields (47).

Step 4: Pointwise convergence of ψ_m to ψ . We prove that the point-wise limit of $\psi_m(\boldsymbol{\sigma})$ exists as $m \rightarrow \infty$ for all $\boldsymbol{\sigma} \neq \mathbf{0}$. Since $\psi_m(\boldsymbol{\sigma}) \geq 0$, it is enough to show that

$$\forall \sigma^\pm > 0 \exists C > 0 \forall \varepsilon > 0 \exists L > 0 \forall \ell \geq L \exists M > 0 \forall m \geq M : \psi_m(\boldsymbol{\sigma}) - \psi_\ell(\boldsymbol{\sigma}) < C\varepsilon. \quad (48)$$

Indeed, it is easy to see that (48) implies that the sequence $(\psi_m(\boldsymbol{\sigma}))_m$ is bounded in m (set $\varepsilon = 1$, and choose $\ell = L$; then $\psi_m(\boldsymbol{\sigma}) \leq \psi_\ell(\boldsymbol{\sigma}) + C$), and that $(\psi_m(\boldsymbol{\sigma}))_m$ can have at most one accumulation point. Therefore, (48) implies that $(\psi_m(\boldsymbol{\sigma}))_m$ is convergent.

To prove (48), we fix any $\boldsymbol{\sigma} \neq \mathbf{0}$, and take any $0 < \varepsilon < \frac{1}{2}$ small enough such that either (32) or (47) applies with $\delta = \varepsilon$. We choose L such that

$$\sigma L \geq \frac{12}{\varepsilon}, \quad \max_{\ell \geq L} \ell V_{\text{eff}}(\ell) < \varepsilon, \quad \max_{\ell \geq \varepsilon L} \ell V(\ell) < \varepsilon^2, \quad (49)$$

where $\sigma = \sigma^+ + \sigma^-$. We take any $\ell \geq L$, set $n_\ell := \lfloor \sigma^+ \ell \rfloor + \lfloor \sigma^- \ell \rfloor$ and $y \in [0, 1]^{n_\ell}$ as a minimiser of $\psi_\ell(\boldsymbol{\sigma})$. We choose M such that $M \geq 3\ell/\varepsilon$ and such that for any $m \geq M$, it holds that

$$\psi_m(\boldsymbol{\sigma}) - \psi_m((1 - \varepsilon)\boldsymbol{\sigma}) \leq C\varepsilon. \quad (50)$$

The existence of such M is guaranteed by (32) or (47). We take any $m > M$, and observe from (50) that (48) holds if

$$\psi_m((1 - \varepsilon)\boldsymbol{\sigma}) - \psi_\ell(\boldsymbol{\sigma}) < C\varepsilon \quad (51)$$

for some C which only depends on $\boldsymbol{\sigma}$.

Next we construct an admissible vector z for the minimisation problem given by $\psi_m((1 - \varepsilon)\boldsymbol{\sigma})$. Such vector should be ordered, have at least

$$n_m := \lfloor (1 - \varepsilon)\sigma^+ m \rfloor + \lfloor (1 - \varepsilon)\sigma^- m \rfloor$$

entries, $z_1 \geq 0$ and the last entry should be smaller than or equal to 1. We construct such z by concatenating $N := \lceil n_m/n_\ell \rceil$ scaled copies of the minimiser y of $\psi_\ell(\boldsymbol{\sigma})$, including a small gap between any consecutive copies;

$$z := \frac{\ell}{m} (y, y + (1 + \frac{\varepsilon}{3}), y + 2(1 + \frac{\varepsilon}{3}), \dots, y + (N - 1)(1 + \frac{\varepsilon}{3})).$$

To show that the final entry satisfies $z_{Nn_\ell} \leq 1$, we first use $\frac{4}{\sigma\ell} \leq \frac{\varepsilon}{3}$ to estimate

$$N - 1 \leq \frac{n_m}{n_\ell} \leq \frac{(1 - \varepsilon)\sigma m}{\sigma\ell - 2} \leq \frac{m}{\ell} \frac{1 - \varepsilon}{1 - \frac{2}{\sigma\ell}} \leq \frac{m}{\ell} (1 - \varepsilon) \left(1 + \frac{4}{\sigma\ell}\right) \leq \frac{m}{\ell} (1 - \varepsilon) \left(1 + \frac{\varepsilon}{3}\right). \quad (52)$$

Then, we obtain by $\frac{\ell}{m} \leq \frac{\varepsilon}{3}$ that

$$z_{Nn_\ell} \leq \frac{\ell}{m} \left(1 + (N - 1)(1 + \frac{\varepsilon}{3})\right) \leq \frac{\varepsilon}{3} + (1 - \varepsilon)(1 + \frac{\varepsilon}{3})^2 < 1.$$

We motivate our choice of z as follows. Each scaled copy of y has interaction energy $\frac{1}{N} \psi_\ell(\boldsymbol{\sigma})(1 + \mathcal{O}(\varepsilon))$. The gaps between neighbouring copies of y allow us to estimate the interdistance (and hence the interaction energy) of any two particles within these copies. For any other pair of particles, we use the number of copies in between them to estimate their interaction energy. More precisely, we estimate

$$\begin{aligned} \psi_m((1 - 4\varepsilon)\boldsymbol{\sigma}) &\leq \frac{1}{m} \sum_{i>j}^{n_m} V_{ij}(m(z_i - z_j)) \\ &\leq N \frac{\ell}{m} \frac{1}{\ell} \sum_{i>j}^{n_\ell} V_{ij}(m \frac{\ell}{m} (y_i - y_j)) + \frac{1}{m} \sum_{k=1}^{N-1} \sum_{j=1}^{N-k} n_\ell^2 V(m \frac{\ell}{m} [\varepsilon + (k - 1)]). \end{aligned} \quad (53)$$

We estimate both terms in the right-hand side of (53) separately. Using (52) and $\frac{\ell}{m} \leq \frac{\varepsilon}{3}$, we have that $N \frac{\ell}{m} < 1$, and thus

$$N \frac{\ell}{m} \frac{1}{\ell} \sum_{i>j}^{n_\ell} V_{ij}(\ell(y_i - y_j)) \leq \psi_\ell(\boldsymbol{\sigma}),$$

where we have used that y is a minimiser of $\psi_\ell(\boldsymbol{\sigma})$. Regarding the second term in the right-hand side of (53), the summand is independent of j , and thus we can estimate the sum over j from

above by multiplication with $N - 1$. Then, estimating the constant in front of the summation over k by

$$(N - 1)n_\ell^2 \leq n_m n_\ell \leq ((1 - \varepsilon)\sigma m)(\sigma \ell) \leq \sigma^2 m \ell,$$

we estimate the second term in the right-hand side of (53) by

$$\begin{aligned} \frac{1}{m} \sum_{k=1}^{N-1} \sum_{j=1}^{N-k} n_\ell^2 V\left(m \frac{\ell}{m} [\varepsilon + (k-1)]\right) &\leq \frac{N-1}{m} n_\ell^2 \left(V(\ell \varepsilon) + \sum_{k=2}^{N-1} V(\ell(k-1)) \right) \\ &\leq \sigma^2 \left(\frac{1}{\varepsilon} \ell \varepsilon V(\ell \varepsilon) + \ell V_{\text{eff}}(\ell) \right), \end{aligned}$$

which, by our choice of L in (49), is bounded by $C\varepsilon$. Collecting our estimates on the right-hand side of (53), it follows directly that (51) holds, which completes the proof of (48). \square

Before proving Γ -convergence in Theorem 4.13, we cite a standard property of Lebesgue points and introduce the dual bounded Lipschitz norm, which, on the interval $[0, 1]$, is equivalent to the narrow topology.

Lemma 4.11 (Rudin, Thm. 7.10). *Let $d \geq 1$ and $f \in L^1(0, 1; \mathbb{R}^d)$. Then, for any Lebesgue point $x \in (0, 1)$ of f and any sequences (A_i) of Lebesgue measurable sets satisfying $A_i \subset [x - \frac{1}{i}, x + \frac{1}{i}]$ and $|A_i| \geq \frac{c}{i}$ for some $c > 0$ independent of i , it holds that*

$$f(x) = \lim_{i \rightarrow \infty} \frac{1}{|A_i|} \int_{A_i} f(y) dy.$$

We define the bounded Lipschitz norm for functions $\varphi : [0, 1] \rightarrow \mathbb{R}$ by

$$\|\varphi\|_{\text{BL}} := \|\varphi\|_\infty + \sup_{x, y \in [0, 1]} \frac{|\varphi(x) - \varphi(y)|}{|x - y|},$$

and the dual bounded Lipschitz norm on the space of signed measures as

$$\|\nu\|_{\text{BL}}^* := \sup_{\|\varphi\|_{\text{BL}}=1} \int_0^1 \varphi d\nu.$$

Lemma 4.12 (Special case of [Dud66, Thm. 18]). *Let $(\mu_n) \subset \mathcal{M}_+([0, 1])$. Then*

$$\mu_n \rightharpoonup \mu \iff \|\mu_n - \mu\|_{\text{BL}}^* \rightarrow 0.$$

Theorem 4.13 (Γ -convergence of E_n in case $\frac{1}{n}\alpha_n \rightarrow \alpha > 0$). *Let $\frac{1}{n}\alpha_n \rightarrow \alpha > 0$, and let V and W satisfy Assumption 4.7. Then E_n Γ -converges to*

$$E(\mu) = \int_0^1 \psi(\rho(x)) dx,$$

where the right-hand side is defined as ∞ if μ is not absolutely continuous (cf. (16)).

Proof. Since Assumption 4.7 is invariant under the scaling $\alpha V(\alpha \cdot)$ and $\alpha W(\alpha \cdot)$ for any $\alpha > 0$, we set $\alpha = 1$ without loss of generality.

We first proof the liminf-inequality (17a). For technical reasons, we assume that (α_n) is strictly increasing as a mapping of \mathbb{N} to $(0, \infty)$, and leave the general case to the end of the proof of (17a). We set $\alpha : (0, \infty) \rightarrow (0, \infty)$ as the linear interpolation between the coordinates $(0, 0)$ and $(n, \alpha_n)_{n \in \mathbb{N}}$, note that the inverse $\alpha^{-1} : (0, \infty) \rightarrow (0, \infty)$ exists, and obtain

$$\alpha(x)/x \xrightarrow{x \rightarrow \infty} 1, \quad \alpha^{-1}(x)/x \xrightarrow{x \rightarrow \infty} 1.$$

Let $\mu \in M([0, 1])$ and $\mu_n \rightharpoonup \mu$ with corresponding particle positions $x^{n, \pm}$ such that $E_n(x^n)$ is bounded uniformly in n . First, we prove that this uniform bound on $E_n(x^n)$ implies regularity on μ^\pm . Indeed, starting from

$$C \geq \liminf_{n \rightarrow \infty} E_n(x^n) \geq \liminf_{n \rightarrow \infty} (E_n^+(x^{n, +}) + E_n^-(x^{n, -}))$$

and using Lemma 4.9 and (31) to estimate

$$\begin{aligned} \liminf_{n \rightarrow \infty} E_n^\pm(x^{n,\pm}) &\geq \liminf_{n \rightarrow \infty} \frac{1}{n^2} \sum_{i=1}^{n^+} \sum_{j=1}^{i-1} \alpha_n V^{**}(\alpha_n(x_i^\pm - x_j^\pm)) \\ &\geq \int_0^1 (V^{**})_{\text{eff}}\left(\frac{1}{\rho^\pm(x)}\right) \rho^\pm(x) dx \geq c(\|\rho^\pm\|_2^2 - C), \end{aligned}$$

we conclude that μ^\pm is absolutely continuous with density $\rho^\pm \in L^2(0,1)$.

Next we estimate $E_n(x^n)$ from below by a sum of $K \in \mathbb{N}$ *independent* cell problems. Given K , we consider the equidistant partition of $[0,1]$ as illustrated in Figure 4, and interpret each interval J_k as a cell. More precisely, we set $J_1 := [0, \frac{1}{K}]$ and $J_k := (\frac{k-1}{K}, \frac{k}{K}]$ for all $2 \leq k \leq K$. For any $1 \leq k \leq K$, we further set

$$n_k^\pm := n\mu_n^\pm(J_k) = \#\{x_i^\pm \in J_k : 1 \leq i \leq n^\pm\}, \quad n_k := n_k^+ + n_k^-.$$

Since $\mu_n^\pm \rightharpoonup \mu^\pm$ and $\rho^\pm \in L^1(0,1)$, it holds that

$$\sigma_k^{n,\pm} := K\mu_n^\pm(J_k) \xrightarrow{n \rightarrow \infty} K\mu^\pm(J_k) =: \sigma_k^\pm, \quad \text{for all } 1 \leq k \leq K. \quad (54)$$

By removing many long range interactions from the energy and exploiting the translation invariance of the interactions, we estimate

$$\begin{aligned} E_n(x^n) &\geq \sum_{k=1}^K \frac{1}{n^2} \sum_{\substack{x_i, x_j \in J_k \\ i > j}} \alpha_n V_{ij}(\alpha_n[x_i - x_j]) \\ &\geq \sum_{k=1}^K \min \left\{ \frac{\alpha_n}{n^2} \sum_{i > j}^{n_k} V_{ij}(\alpha_n[\tilde{x}_i - \tilde{x}_j]) : \tilde{x}_i \in \overline{J_k} \quad \forall 1 \leq i \leq n_k \right\} \\ &= \frac{\alpha_n^2}{n^2} \frac{1}{K} \sum_{k=1}^K \min \left\{ \frac{K}{\alpha_n} \sum_{i > j}^{n_k} V_{ij}\left(\frac{\alpha_n}{K}[y_i - y_j]\right) : y_i \in [0,1] \quad \forall 1 \leq i \leq n_k \right\}, \end{aligned}$$

where we define the value of the minimisation problem to be 0 when $n_k = 0$.

Next, we change variables to bound these minimisation problems from below in terms of the cell problem (28b). We fix k , and set

$$m_n := \frac{\alpha_n}{K}.$$

It remains to define $\tilde{\sigma}_k^{m,\pm}$ such that

$$n_k = m_n \tilde{\sigma}_k^{m_n,+} + m_n \tilde{\sigma}_k^{m_n,-} \quad (55)$$

for all $n \in \mathbb{N}$. Motivated by

$$n_k = \frac{n}{K} \sigma_k^n = m_n \frac{1}{m_n} \frac{n}{K} \sigma_k^{n,+} + m_n \frac{1}{m_n} \frac{n}{K} \sigma_k^{n,-}$$

and recalling that $n = \alpha^{-1}(\alpha_n) = \alpha^{-1}(Km_n)$, we set

$$\tilde{\sigma}_k^{m,\pm} := \frac{\alpha^{-1}(Km)}{Km} \sigma_k^{[\alpha^{-1}(Km)],\pm}, \quad \tilde{\sigma}_k^m := \tilde{\sigma}_k^{m,+} + \tilde{\sigma}_k^{m,-} \quad \text{for all } m > 0.$$

By construction, (55) holds for $m = m_n$ and $\tilde{\sigma}_k^{m,\pm} \rightarrow \sigma_k^\pm$ as $m \rightarrow \infty$. We obtain

$$\begin{aligned}
& \liminf_{n \rightarrow \infty} \min \left\{ \frac{K}{\alpha_n} \sum_{i>j}^{n_k} V_{ij} \left(\frac{\alpha_n}{K} [y_i - y_j] \right) : y_i \in [0, 1] \quad \forall 1 \leq i \leq n_k \right\} \\
&= \liminf_{n \rightarrow \infty} \min \left\{ \frac{1}{m_n} \sum_{i>j}^{m_n \tilde{\sigma}_k^{m_n}} V_{ij} (m_n [y_i - y_j]) : y_i \in [0, 1] \quad \forall 1 \leq i \leq m_n \tilde{\sigma}_k^{m_n} \right\} \\
&\geq \liminf_{m \rightarrow \infty} \min \left\{ \frac{1}{m} \sum_{i>j}^{\lfloor m \tilde{\sigma}_k^{m,+} \rfloor + \lfloor m \tilde{\sigma}_k^{m,-} \rfloor} V_{ij} (m [y_i - y_j]) : \right. \\
&\quad \left. 0 \leq y_1^+ \leq \dots \leq y_{\lfloor m \tilde{\sigma}_k^{m,+} \rfloor}^+ \leq 1, 0 \leq y_1^- \leq \dots \leq y_{\lfloor m \tilde{\sigma}_k^{m,-} \rfloor}^- \leq 1 \right\} \\
&= \liminf_{m \rightarrow \infty} \psi_m(\tilde{\sigma}_k^m).
\end{aligned}$$

Applying Lemma 4.10.(vii), we obtain

$$\liminf_{n \rightarrow \infty} E_n(\mu_n) \geq \frac{1}{K} \sum_{k=1}^K \psi(\sigma_k) \geq \frac{1}{K} \sum_{k=1}^K (M \wedge \psi(\sigma_k)). \quad (56)$$

for any $M > 0$.

Finally, we derive (17a) from (56) by first passing to the limit $K \rightarrow \infty$ and then $M \rightarrow \infty$. To this aim, we set

$$\rho_K^\pm(x) := \sum_{k=1}^K \left(K \int_{J_k} \rho^\pm(y) dy \right) \mathbb{1}_{J_k}(x) = \sum_{k=1}^K \sigma_k^\pm \mathbb{1}_{J_k}(x)$$

and observe that

$$\frac{1}{K} \sum_{k=1}^K (M \wedge \psi(\sigma_k)) = \int_0^1 [M \wedge \psi(\rho_K(x))] dx. \quad (57)$$

First, by Lemma 4.11, $\rho_K \rightarrow \rho$ pointwise a.e. on $(0, 1)$ as $K \rightarrow \infty$. Second, by Lemma 4.10.(v),(vi), it holds that $M \wedge \psi : [0, \infty)^2 \rightarrow \mathbb{R}$ is uniformly continuous. Together, these statements imply

$$M \wedge \psi(\rho_K(x)) \xrightarrow{K \rightarrow \infty} M \wedge \psi(\rho(x)) \quad \text{for a.e. } x \in (0, 1).$$

Hence, by the Dominated Convergence Theorem, we can pass to the limit $K \rightarrow \infty$ in (57) to obtain

$$\frac{1}{K} \sum_{k=1}^K (M \wedge \psi(\sigma_k)) \xrightarrow{K \rightarrow \infty} \int_0^1 (M \wedge \psi(\rho(x))) dx.$$

Then, using the Monotone Convergence Theorem, we pass to the limit $M \rightarrow \infty$ to obtain

$$\int_0^1 (M \wedge \psi(\rho(x))) dx \xrightarrow{M \rightarrow \infty} \int_0^1 \psi(\rho(x)) dx = E(\mu),$$

which completes the proof of the liminf-inequality (17a) under the assumption that (α_n) is increasing.

In the general case where (α_n) is not increasing, we consider any subsequence (α_{n_k}) , and extract another subsequence which is increasing. Such a subsequence always exists, because $\alpha_n \rightarrow \infty$ as $n \rightarrow \infty$. The arguments above apply also to this increasing subsequence, and since the limit in (54) and the lower bound in (56) do not depend on the choice of the subsequence, we conclude that (17a) holds for any (α_n) with $\frac{1}{n} \alpha_n \rightarrow 1$.

The second part of the proof establishes the limsup-inequality (17b). Let $\mu \in M([0, 1])$ such that $E(\mu)$ is finite. Then, by Lemma 4.10.(v) it follows that $\rho \in L^2(0, 1)$. Next we show, by the usual density arguments, that it suffices to construct a recovery sequence in (17b) only for $\rho \in C([0, 1]) \cap M([0, 1])$. To prove this, we take $\rho \in L^2(0, 1) \cap M([0, 1])$ arbitrarily and construct $(\rho_\varepsilon) \subset C([0, 1]) \cap M([0, 1])$ such that $\rho_\varepsilon \rightarrow \rho$ as $\varepsilon \rightarrow 0$ and

$$\limsup_{\varepsilon \rightarrow 0} E(\rho_\varepsilon) \leq E(\rho). \quad (58)$$

We first assume that $\boldsymbol{\rho} \in L^\infty([0, 1]) \cap M([0, 1])$. We take any $(\boldsymbol{\rho}_\varepsilon) \subset C([0, 1]) \cap M([0, 1])$ such that $\boldsymbol{\rho}_\varepsilon \rightarrow \boldsymbol{\rho}$ as $\varepsilon \rightarrow 0$ both in $L^2(0, 1)$ and pointwise a.e. on $(0, 1)$. To show that such a choice is possible, take for example $\tilde{\rho}_\varepsilon^\pm := \eta_\varepsilon * \rho^\pm \in C^\infty(\mathbb{R})$, where η_ε is the usual mollifier. Note that the non-negativity and unit mass condition are satisfied, but that $\text{supp } \tilde{\rho}_\varepsilon$ may not be contained in $[0, 1]$. This is easily fixed by setting

$$\rho_\varepsilon^\pm := \tilde{\rho}_\varepsilon^\pm|_{(0,1)} + \int_{\mathbb{R} \setminus (0,1)} \tilde{\rho}_\varepsilon^\pm.$$

By construction, $(\boldsymbol{\rho}_\varepsilon) \subset C([0, 1]) \cap M([0, 1])$ and $\boldsymbol{\rho}_\varepsilon \rightarrow \boldsymbol{\rho}$ in $L^2(0, 1)$ as $\varepsilon \rightarrow 0$. By extracting a subsequence, we then also have $\boldsymbol{\rho}_\varepsilon \rightarrow \boldsymbol{\rho}$ pointwise a.e. on $(0, 1)$. To check that (58) is satisfied, we observe that $\|\boldsymbol{\rho}_\varepsilon\|_\infty \leq \|\boldsymbol{\rho}\|_\infty + \frac{1}{2}$. Then, by Lemma 4.10.(v),(vi), ψ is uniformly continuous on the levelset $\{\psi \leq \|\boldsymbol{\rho}\|_\infty + \frac{1}{2}\}$, and thus we obtain (58) by applying the Dominated Convergence Theorem.

To complete the density argument, we take any $\boldsymbol{\rho} \in L^2([0, 1]) \cap M([0, 1])$, and construct $(\boldsymbol{\rho}_\varepsilon) \subset L^\infty([0, 1]) \cap M([0, 1])$ which converges narrowly to $\boldsymbol{\rho}$ and satisfies (58). Let $A^\pm := \{\rho^\pm \leq 3\}$ and $A = A^+ \cap A^-$. We note that $|A| \geq \frac{1}{3}$, and set

$$\rho_\varepsilon^\pm := (\rho^\pm \wedge \frac{1}{\varepsilon}) \vee (m_\varepsilon^\pm \mathbb{1}_A),$$

where we set $0 \leq m_\varepsilon^\pm \leq 3$ such that $\int_0^1 \rho_\varepsilon^\pm = \int_0^1 \rho^\pm$. We note that $m_\varepsilon^\pm \rightarrow 0$ as $\varepsilon \rightarrow 0$, and hence $\boldsymbol{\rho}_\varepsilon \rightarrow \boldsymbol{\rho}$ both in $L^2(0, 1)$ and pointwise a.e. on $(0, 1)$. In particular, $\boldsymbol{\rho}_\varepsilon$ is uniformly bounded on A , and $\boldsymbol{\rho}_\varepsilon \nearrow \boldsymbol{\rho}$ pointwise a.e. on A^c . Hence, by using both the Dominated and Monotone Convergence Theorems, we obtain

$$E(\boldsymbol{\rho}_\varepsilon) = \int_A \psi(\boldsymbol{\rho}_\varepsilon) + \int_{A^c} \psi(\boldsymbol{\rho}_\varepsilon) \xrightarrow{\varepsilon \rightarrow 0} \int_A \psi(\boldsymbol{\rho}) + \int_{A^c} \psi(\boldsymbol{\rho}) = E(\boldsymbol{\rho}).$$

To prove (17b), it remains to construct a recovery sequence (\bar{x}^n) for any $\boldsymbol{\rho} \in C([0, 1]) \cap M([0, 1])$. We do this by a slight modification of the usual density argument. First, we approximate $\boldsymbol{\rho}$ by $\boldsymbol{\rho}^\ell$ similarly as in the proof of Theorem 4.6, i.e., we set

$$K_\ell = 2^\ell, \quad \varepsilon_\ell = \sqrt{\frac{1}{K_\ell} + \frac{1}{4}} - \frac{1}{2} = \frac{1}{2}(\sqrt{2^{2-\ell} + 1} - 1) \quad \text{for } \ell = 1, 2, \dots, \quad (59)$$

and take the intervals I_k and J_k of size $\varepsilon_\ell > 0$ and $\varepsilon_\ell(1 + \varepsilon_\ell) > 0$ respectively, as in Figure 4. Then, as in (24) we set

$$\boldsymbol{\rho}^\ell = \sum_{k=1}^{K_\ell} \sigma_k \mathbb{1}_{I_k}, \quad \text{where } \sigma_k := \frac{1}{\varepsilon_\ell} \int_{J_k} \boldsymbol{\rho} \quad \text{for } k = 1, \dots, K_\ell.$$

Since $\boldsymbol{\rho} \in C([0, 1])$, it holds that $\boldsymbol{\rho}^\ell \rightarrow \boldsymbol{\rho}$ in $L^2(0, 1)$ as $\ell \rightarrow \infty$ and $\|\boldsymbol{\rho}^\ell\|_\infty \leq (1 + \varepsilon_\ell)\|\boldsymbol{\rho}\|_\infty$. Hence, along a subsequence ℓ_j , $\boldsymbol{\rho}^{\ell_j} \rightarrow \boldsymbol{\rho}$ pointwise a.e. on $(0, 1)$. Then, by Lemma 4.10.(v),(vi), we have $\psi(\boldsymbol{\rho}^{\ell_j}) \rightarrow \psi(\boldsymbol{\rho})$ pointwise a.e. on $(0, 1)$ as $j \rightarrow \infty$, and $\psi(\boldsymbol{\rho}^\ell)$ uniformly bounded in ℓ . By the Dominated Convergence Theorem, we conclude that

$$E(\boldsymbol{\rho}^{\ell_j}) \xrightarrow{j \rightarrow \infty} E(\boldsymbol{\rho}). \quad (60)$$

Given $\ell \in \mathbb{N}$, we construct a ‘recovery sequence’ (x^n) for $\boldsymbol{\rho}^\ell$ by concatenating the minimisers of the cell problems (28b) corresponding to each I_k . We prove that

$$\limsup_{n \rightarrow \infty} E_n(x^n) \leq E(\boldsymbol{\rho}^\ell), \quad (61)$$

but do not require that $\boldsymbol{\mu}_n \rightharpoonup \boldsymbol{\rho}^\ell$ as $n \rightarrow \infty$. Hence, (x^n) may not be a recovery sequence for $\boldsymbol{\rho}^\ell$. Instead, we construct (x^n) such that in the joint limit $n \rightarrow \infty$ and $\ell \rightarrow \infty$, it holds that (x^n) (which also depends on ℓ) converges to $\boldsymbol{\rho}$. We prove this at the end of the proof by a diagonal argument on (60) and (61).

Given $\ell \in \mathbb{N}$, we construct x^n and show that it satisfies (61). Since ℓ is fixed, we remove it from the notation whenever convenient. Given $n \in \mathbb{N}$, we set $\boldsymbol{\sigma} := \int_0^1 \boldsymbol{\rho}^\ell$, note that $\sigma^+ + \sigma^- = 1$, and choose $n^\pm \in \mathbb{N} \cup \{0\}$ such that $|n^\pm - n\sigma^\pm| \leq \frac{1}{2}$ and $n^+ + n^- = n$. Recalling that $\varepsilon > 0$ is such

that $K\varepsilon(1+\varepsilon) = 1$, we divide the positive and negative particles over the intervals I_k by choosing $n_k^\pm \in \mathbb{N} \cup \{0\}$ such that $\sum_{k=1}^K n_k^\pm = n^\pm$ and $|n_k^\pm - \varepsilon n \sigma_k^\pm| \leq 1$. An example of such a choice is given in the proof of Theorem 4.6. We further set the average density of the particles at I_k as

$$\sigma_k^{n,\pm} := \frac{1}{\varepsilon \alpha_n} n_k^\pm,$$

and observe that

$$\left| \frac{\alpha_n}{n} \sigma_k^{n,\pm} - \sigma_k^\pm \right| \leq \frac{1}{\varepsilon n} \quad \text{for } 1 \leq k \leq K. \quad (62)$$

We set $y^k \in \mathbb{R}^{n_k}$ as a minimiser of $\psi_{\varepsilon \alpha_n}(\sigma_k^n)$, and observe from (28b) that

$$\psi_{\varepsilon \alpha_n}(\sigma_k^n) = \frac{1}{\varepsilon \alpha_n} \sum_{i>j}^{\varepsilon \alpha_n \sigma_k^n} V_{ij}(\varepsilon \alpha_n (y_i - y_j)) = \frac{1}{\varepsilon \alpha_n} \sum_{i>j}^{n_k} V_{ij}(\varepsilon \alpha_n (y_i - y_j)).$$

Finally, we set the recovery sequence x^n by scaling and translating the particle positions y^k from the cell problem to I_k . More precisely, we set

$$\tilde{x}_i^k := \varepsilon y_i^k + \varepsilon(1+\varepsilon)(k-1) \quad \text{for } i = 1, \dots, n_k, \quad \text{and} \quad x^n := (\tilde{x}^1, \dots, \tilde{x}^K). \quad (63)$$

To prove (61), we follow a similar argument as the one starting at (53). We expand

$$\begin{aligned} E_n(x^n) &= \frac{\alpha_n}{n^2} \sum_{i>j}^n V_{ij}(\alpha_n(x_i - x_j)) \\ &= \sum_{k=1}^K \frac{\alpha_n}{n^2} \sum_{i>j}^{n_k} V_{ij}(\alpha_n(\tilde{x}_i^k - \tilde{x}_j^k)) + 2 \sum_{l=1}^{K-1} \sum_{k=1}^{K-l} \frac{\alpha_n}{n^2} \sum_{i=1}^{n_{k+l}} \sum_{j=1}^{n_k} V_{ij}(\alpha_n(\tilde{x}_i^{k+l} - \tilde{x}_j^k)). \end{aligned} \quad (64)$$

By construction and Lemma 4.10.(vii), we pass to the limit $n \rightarrow \infty$ in the first term in the right-hand side of (64) by

$$\begin{aligned} \sum_{k=1}^K \frac{\alpha_n}{n^2} \sum_{i>j}^{n_k} V_{ij}(\alpha_n(\tilde{x}_i^k - \tilde{x}_j^k)) &= \frac{\alpha_n^2}{n^2} \sum_{k=1}^K \varepsilon \frac{1}{\varepsilon \alpha_n} \sum_{i>j}^{n_k} V_{ij}(\varepsilon \alpha_n (y_i^k - y_j^k)) = \varepsilon \sum_{k=1}^K \psi_{\varepsilon \alpha_n}(\sigma_k^n) \\ &\xrightarrow{n \rightarrow \infty} \varepsilon \sum_{k=1}^K \psi(\sigma_k) = \int_0^1 \psi(\rho^\ell) = E(\rho^\ell). \end{aligned}$$

It remains to show that the second term in the right-hand side of (64) converges to 0 as $n \rightarrow \infty$. Using that $\tilde{x}_i^{k+l} - \tilde{x}_j^k \geq \varepsilon^2 + (l-1)\varepsilon$ and $V_{ij} \leq V$, we estimate

$$\begin{aligned} \sum_{l=1}^{K-1} \sum_{k=1}^{K-l} \frac{\alpha_n}{n^2} \sum_{i=1}^{n_{k+l}} \sum_{j=1}^{n_k} V_{ij}(\alpha_n(\tilde{x}_i^{k+l} - \tilde{x}_j^k)) &\leq \sum_{l=1}^{K-1} \sum_{k=1}^{K-l} \frac{n_{k+l} n_k}{n^2} \alpha_n V(\alpha_n \varepsilon^2 + \alpha_n(l-1)\varepsilon) \\ &\leq \sum_{l=1}^{K-1} \sum_{k=1}^{K-l} \frac{(\varepsilon n \sigma_{k+l} + 2)(\varepsilon n \sigma_k + 2)}{n^2} \alpha_n V(\alpha_n \varepsilon^2 + \alpha_n(l-1)\varepsilon) \\ &\leq K \left[\max_{1 \leq k \leq K} \sigma_k \right]^2 \varepsilon^2 (1 + \mathcal{O}(n^{-1})) (\alpha_n V(\alpha_n \varepsilon^2) + \alpha_n V_{\text{eff}}(\alpha_n \varepsilon)). \end{aligned} \quad (65)$$

Since the constants ε , K and $\max_k \sigma_k$ are fixed by the choice of ρ^ℓ , it follows from (27) that (65) converges to 0 as $n \rightarrow \infty$.

Finally, we complete the proof of (17b) for $\rho \in C([0, 1]) \cap M([0, 1])$ by constructing the sequence \bar{x}^n . For any $\ell \geq 1$, let $x_\ell^n \in \mathbb{R}^n$ be the sequence constructed in (63) for which (61) holds. Then, by a diagonal argument, we find from (60) and (61) that

$$\bar{x}^n := x_{\ell_{j_n}}^n \quad \text{satisfies} \quad \limsup_{n \rightarrow \infty} E_n(\bar{x}^n) \leq E(\rho)$$

for any non-decreasing sequence $j_n \rightarrow \infty$ as $n \rightarrow \infty$ provided that j_n is small enough with respect to n . We choose j_n such that $K^n := K_{\ell_{j_n}}$ (defined in (59), together with $\varepsilon^n := \varepsilon_{\ell_{j_n}}$) satisfies $\frac{1}{n} K^n \rightarrow 0$ as $n \rightarrow \infty$. For such choice, we prove that the recovery sequence satisfies $\bar{\mu}_n \rightarrow \rho$.

In the estimate below, we simplify notation by writing I_k , J_k , σ_k , n_k^\pm and σ_k^n for the objects corresponding to the construction of x_ℓ^n in (63) for $\ell = \ell_{j_n}$. By Lemma 4.12, the convergence of the recovery sequence follows from (62) by

$$\begin{aligned} \|\bar{\mu}_n^\pm - \rho^\pm\|_{\text{BL}}^* &= \sup_{\|\varphi\|_{\text{BL}}=1} \int_0^1 \varphi d(\bar{\mu}_n^\pm - \rho^\pm) = \sup_{\|\varphi\|_{\text{BL}}=1} \sum_{k=1}^{K^n} \left[\int_{J_k} \varphi d\bar{\mu}_n^\pm - \int_{J_k} \varphi d\rho^\pm \right] \\ &\leq \sup_{\|\varphi\|_{\text{BL}}=1} \sum_{k=1}^{K^n} \left[\left(\sup_{J_k} \varphi \right) \frac{n_k^\pm}{n} - \left(\inf_{J_k} \varphi \right) \varepsilon^n \sigma_k^\pm \right] \\ &= \sup_{\|\varphi\|_{\text{BL}}=1} \sum_{k=1}^{K^n} \left[\left(\sup_{J_k} \varphi \right) \varepsilon^n \left(\frac{\alpha_n}{n} \sigma_k^{n,\pm} - \sigma_k^\pm \right) + \left(\sup_{J_k} \varphi - \inf_{J_k} \varphi \right) \varepsilon^n \sigma_k^\pm \right] \\ &\leq K^n \varepsilon^n \frac{1}{\varepsilon^n n} + \sum_{k=1}^{K^n} |J_k| \varepsilon^n \sigma_k^\pm = \frac{K^n}{n} + \varepsilon^n (1 + \varepsilon^n) \sigma^\pm \xrightarrow{n \rightarrow \infty} 0. \quad \square \end{aligned}$$

5. Γ -CONVERGENCE OF E_n IN THE CASE $\gamma_n \rightarrow \infty$

The parameter regime $\gamma_n \rightarrow \infty$ of the energy E_n in (2) describes a scenario where the external forcing is strong enough for the positive particles to cluster at the left barrier (and the negative particles to cluster at the right barrier) on a length-scale asymptotically smaller than 1. In order to obtain a useful limit, it is therefore necessary to rescale $x^{n,\pm}$ to fit to this length-scale. It is shown in [vMMP14] that a sensible rescaling is given by $\hat{x}^{n,+} := \gamma_n x^{n,+}$. We rescale the negative particles similarly, and for convenience later on, we introduce simultaneously the affine variable transformation

$$\hat{x}_i^- := \gamma_n (1 - x_{n^-+1-i}^-), \quad i = 1, \dots, n^-.$$

A result of this variable transformation is that $0 \leq \hat{x}_1^\pm < \dots < \hat{x}_{n^\pm}^\pm \leq \gamma_n$. We rescale the energy as

$$\begin{aligned} \hat{E}_n(\hat{x}^{n,+}, \hat{x}^{n,-}) &:= \frac{1}{\gamma_n} E_n \left(\frac{\hat{x}^{n,+}}{\gamma_n}, \frac{1}{\gamma_n} (1 - \hat{x}_{n^-+1-i}^-)_{i=1}^{n^-} \right) \\ &= \frac{1}{n^2} \sum_{i=1}^{n^+} \sum_{j=1}^{i-1} \hat{\alpha}_n V(\hat{\alpha}_n (\hat{x}_i^+ - \hat{x}_j^+)) + \frac{1}{n^2} \sum_{i=1}^{n^-} \sum_{j=1}^{i-1} \hat{\alpha}_n V(\hat{\alpha}_n (\hat{x}_i^- - \hat{x}_j^-)) \\ &\quad + \frac{1}{n^2} \sum_{i=1}^{n^+} \sum_{j=1}^{n^-} \hat{\alpha}_n W(\hat{\alpha}_n (\gamma_n - \hat{x}_i^+ - \hat{x}_j^-)) + \frac{1}{n} \sum_{i=1}^{n^+} \hat{x}_i^+ + \frac{1}{n} \sum_{i=1}^{n^-} \hat{x}_i^-, \end{aligned}$$

where

$$\hat{\alpha}_n = \alpha_n / \gamma_n.$$

We observe that \hat{E}_n consists of the components

$$\begin{aligned} \hat{E}_n^\pm(\hat{x}^{n,\pm}) &:= \frac{1}{n^2} \sum_{i=1}^{n^\pm} \sum_{j=1}^{i-1} \hat{\alpha}_n V(\hat{\alpha}_n (\hat{x}_i^\pm - \hat{x}_j^\pm)) + \frac{1}{n} \sum_{i=1}^{n^\pm} \hat{x}_i^\pm, \\ \hat{E}_n^{+-}(\hat{x}^{n,+}, \hat{x}^{n,-}) &:= \frac{1}{n^2} \sum_{i=1}^{n^+} \sum_{j=1}^{n^-} \hat{\alpha}_n W(\hat{\alpha}_n (\gamma_n - \hat{x}_i^+ - \hat{x}_j^-)). \end{aligned}$$

We note that \hat{E}_n^+ and \hat{E}_n^- are the same energies when $n^+ = n^-$. Moreover, Γ -convergence of \hat{E}_n^\pm was first proven in [GPPS13] for all scaling regimes of $\hat{\alpha}_n$, and in §4 we extend this result by relaxing the assumptions on V ; see Table 3. The Γ -limit is given by

$$\hat{E}^\pm(\hat{\mu}^\pm) = \hat{E}^{(\text{int})}(\hat{\mu}^\pm) + \int_0^\infty x d\hat{\mu}^\pm(x), \quad (66)$$

Regime	properties of V
$\hat{\alpha}_n \rightarrow \hat{\alpha} > 0$	$V = V_{\text{sing}} + V_{\text{reg}} \in L^1(\mathbb{R})$, where $V_{\text{reg}} \in C_b(\mathbb{R})$ is even, and $V_{\text{sing}} \in L^1(\mathbb{R})$ is even, non-negative and non-increasing on $(0, \infty)$;
$1 \ll \hat{\alpha}_n \ll n$	V satisfies Assumption 4.4 with $W = 0$;
$\frac{\hat{\alpha}_n}{n} \rightarrow \hat{\alpha}$	$V : \mathbb{R} \setminus \{0\} \rightarrow [0, \infty)$ is even, and convex on $(0, \infty)$. Moreover, $V(0) := \lim_{x \rightarrow 0} V(x) \in [0, \infty]$ and $\int_1^\infty V < \infty$.

TABLE 3. Properties of V for which \hat{E}_n^\pm is Γ -convergent.

where the expression of $\hat{E}^{(\text{int})}$ depends on the asymptotic behaviour of $\hat{\alpha}_n$ (see Table 4). Since boundedness of \hat{E}_n^\pm forces the bulk of the particles to remain in a bounded interval, the second component of \hat{E}_n (given by \hat{E}_n^{+-}) vanishes in the limit $n \rightarrow \infty$ given that W satisfies Assumption 5.1. Theorem 5.2 makes this statement precise.

Assumption 5.1 (Properties of W in case $\gamma_n \rightarrow \infty$). *$W : \mathbb{R} \rightarrow [0, \infty]$ is even, and satisfies $W(x) \leq \frac{C}{x}$ for all $x \geq 1$ and $C > 0$ independent of x .*

We adopt the same notation to rewrite E_n in terms of the measures $(\hat{\mu}_n^+, \hat{\mu}_n^-) =: \hat{\mu}_n$ given by (3).

Theorem 5.2 (Γ -convergence of \hat{E}_n in case $\gamma_n \rightarrow \infty$). *Let $\gamma_n \rightarrow \infty$, and let W satisfy Assumption 5.1. Let $(\hat{\alpha}_n)$ be as in any of the three scaling regimes outlined in Table 3, and let V satisfy the corresponding assumption. Then, any sequence $(\hat{\mu}_n) \subset M([0, \infty))$ satisfying $\hat{E}_n(\hat{\mu}_n) \leq C$ for some n -independent $C > 0$ is compact in the narrow topology. Moreover, \hat{E}_n Γ -converges to $\hat{E}(\hat{\mu}) = \hat{E}^+(\hat{\mu}^+) + \hat{E}^-(\hat{\mu}^-)$, where \hat{E}^\pm is given by (66) and Table 4.*

Proof. Let $\hat{E}_n(\hat{\mu}_n) \leq C$. Since $W \geq 0$ and V is bounded from below, it holds that

$$\hat{E}_n(\hat{\mu}_n) \geq \hat{\alpha}_n \frac{(n^+)^2 + (n^-)^2 - n}{2n^2} (\inf V) + \int_0^\infty x d(\hat{\mu}_n^+ + \hat{\mu}_n^-)(x). \quad (67)$$

We note from Table 3 that the first term in the right-hand side of (67) is bounded from below. Hence, (67) implies that the first moments of $\hat{\mu}_n^+$ and $\hat{\mu}_n^-$ are uniformly bounded; we conclude compactness of $\hat{\mu}_n$.

Since $W \geq 0$, we obtain the liminf-inequality (17a) from the Γ -convergence of \hat{E}_n^\pm by

$$\liminf_{n \rightarrow \infty} \hat{E}_n(\hat{\mu}_n) \geq \liminf_{n \rightarrow \infty} \hat{E}_n^+(\hat{\mu}_n^+) + \liminf_{n \rightarrow \infty} \hat{E}_n^-(\hat{\mu}_n^-) \geq \hat{E}^+(\hat{\mu}^+) + \hat{E}^-(\hat{\mu}^-) = \hat{E}(\hat{\mu}).$$

We prove the limsup-inequality (17b) by an analogous argument, relying on the claim that

$$\hat{E}_n^{+-}(\hat{\mu}_n) \xrightarrow{n \rightarrow \infty} 0, \quad (68)$$

Regime	$\hat{E}^{(\text{int})}(\hat{\mu})$
$\hat{\alpha}_n \rightarrow \hat{\alpha}$	$\frac{1}{2} \iint_{[0, \infty)^2} \hat{\alpha} V(\hat{\alpha}(x - y)) d(\hat{\mu} \otimes \hat{\mu})(x, y)$
$1 \ll \hat{\alpha}_n \ll n$	$\left(\int_0^\infty V \right) \int_0^\infty \hat{\rho}(x)^2 dx$
$\frac{\hat{\alpha}_n}{n} \rightarrow \hat{\alpha}$	$\int_0^\infty \hat{\alpha} V_{\text{eff}}\left(\frac{\hat{\alpha}}{\hat{\rho}(x)}\right) \hat{\rho}(x) dx$

TABLE 4. Expressions for $\hat{E}^{(\text{int})}$, the interaction part of the limit energy \hat{E}^\pm defined in (66). In the regimes where $\hat{\alpha}_n \gg 1$, the expressions are valid when $\hat{\mu}$ is absolutely continuous (see (16)) with density $\hat{\rho} \in L^1(0, 1)$; otherwise $\hat{E}^{(\text{int})}(\hat{\mu}) = \infty$. Note the resemblance with Table 1.

where $\hat{\mu}_n$ consists of any recovery sequence $\hat{\mu}_n^\pm$ related to the Γ -convergence of \hat{E}_n^\pm . These recovery sequences are constructed explicitly only for $\hat{\mu}^\pm$ smooth enough, including $\hat{\mu}^\pm$ having bounded support. The case for general $\hat{\mu}^\pm$ is treated by a diagonal argument, relying on upper semi-continuity of \hat{E}^\pm . Hence, for any $\hat{\mu} \in M([0, \infty))$ with $\hat{E}(\hat{\mu})$ bounded, we choose the recovery sequences $(\hat{x}^{n,+})$ and $(\hat{x}^{n,-})$ such that

$$\hat{x}_{n+}^+ + \hat{x}_{n-}^- \leq \frac{1}{2}\gamma_n.$$

Then, the claim (68) follows from

$$\begin{aligned} \hat{E}_n^{+-}(\hat{\mu}_n) &= \frac{1}{n^2} \sum_{i=1}^{n^+} \sum_{j=1}^{n^-} \hat{\alpha}_n W(\hat{\alpha}_n(\gamma_n - \hat{x}_i^+ - \hat{x}_j^-)) \\ &\leq \frac{1}{n^2} \sum_{i=1}^{n^+} \sum_{j=1}^{n^-} \hat{\alpha}_n \frac{C}{\hat{\alpha}_n(\gamma_n - (\hat{x}_i^+ + \hat{x}_j^-))} \leq \frac{1}{n^2} \sum_{i=1}^{n^+} \sum_{j=1}^{n^-} \frac{2C}{\gamma_n} \leq \frac{C}{\gamma_n} \xrightarrow{n \rightarrow \infty} 0. \quad \square \end{aligned}$$

6. EVOLUTIONARY CONVERGENCE OF THE GRADIENT FLOW OF E_n IN THE CASE $\alpha_n \rightarrow \alpha > 0$

The starting point in this section is the gradient flow of E_n given by (7) in the scaling regime $\alpha_n \rightarrow \alpha > 0$. The main result (Theorem 6.7) of this section is an evolutionary convergence result of the gradient flows of E_n to the gradient flow of the Γ -limit E as $n \rightarrow \infty$. The proof strategy is to apply the setting of gradient flows with λ -convex energies in [AGS08, Chap. 4] and [DS10] (§6.1) to the gradient flow of E_n (§6.2).

6.1. Preliminaries on gradient flows of λ -convex energies. We summarise a simplified version of the results in [AGS08, Chap. 4] and [DS10]. Let (X, d) be a complete, separable, non-positively curved (see (70)), sequentially compact metric space. We call a curve $x : [0, 1] \rightarrow X$ a (constant speed) *geodesic* if

$$d(x(s), x(t)) = |t - s|d(x(0), x(1)) \quad \text{for all } 0 \leq s \leq t \leq 1. \quad (69)$$

We consider any $\phi : X \rightarrow \mathbb{R} \cup \{\infty\}$ with non-empty domain

$$D(\phi) := \{x \in X : \phi(x) < \infty\},$$

and assume that ϕ is λ -convex for some $\lambda \in \mathbb{R}$, i.e., every couple of points $x_0, x_1 \in D(\phi)$ can be connected by a geodesic x_t along which

$$\phi(x_t) \leq (1-t)\phi(x_0) + t\phi(x_1) - \frac{1}{2}\lambda t(1-t)d(x_0, x_1)^2 \quad \text{for all } 0 \leq t \leq 1.$$

In particular, (X, d) being *non-positively curved* means that

$$x \mapsto \frac{1}{2}d(x, y)^2 \quad \text{is } 1\text{-convex for any } y \in X. \quad (70)$$

We say that $x : (0, \infty) \rightarrow X$ is an *absolutely continuous curve* if there exists an $f \in L^1(0, \infty)$ such that

$$d(x(s), x(t)) \leq \int_s^t f(\tau) d\tau \quad \text{for all } 0 < s \leq t < \infty.$$

We denote by $AC(0, \infty; X)$ the space of absolutely continuous curves.

Given $x_0 \in X$, we say that a curve $x \in AC_{\text{loc}}(0, \infty; X)$ is a *solution* to the *evolution variational inequality* if it satisfies

$$\frac{1}{2} \frac{d}{dt} d(x(t), y)^2 + \frac{\lambda}{2} d(x(t), y)^2 + \phi(x(t)) \leq \phi(y), \quad \text{for a.e. } t > 0, \text{ and all } y \in X, \quad (71)$$

and $x(t) \rightarrow x_0$ as $t \rightarrow 0$.

Theorem 6.1 (Gradient flows [AGS08, Thm. 4.0.4]). *Let (X, d) be a complete, separable, non-positively curved, sequentially compact metric space. Let $\phi : X \rightarrow \mathbb{R}$ with $D(\phi) \neq \emptyset$ be λ -convex for some $\lambda \in \mathbb{R}$. Then for any $x_0 \in \overline{D(\phi)}$, the evolution variational inequality (71) has a unique solution.*

Part of the complete statement of [AGS08, Thm. 4.0.4] characterises the solution to the evolution variational inequality as the limit of the solutions to the corresponding time-discretised minimising movement scheme as the time step converges to 0. This is the motivation to call the solution to the evolution variational inequality a gradient flow.

Note that in the setting of the following theorem, (X, d) need not be non-positively curved.

Theorem 6.2 (Stability of gradient flows [DS10, Thm. 2.17]). *Let $\lambda \in \mathbb{R}$ and (X, d) be a complete, separable, sequentially compact metric space. Let $\phi_n : X \rightarrow \mathbb{R} \cup \{\infty\}$ be a sequence of λ -convex functionals, which Γ -converges (with respect to the metric d) to $\phi : X \rightarrow \mathbb{R} \cup \{\infty\}$, where $D(\phi) \neq \emptyset$. Let $x_\circ^n \in \overline{D\phi_n}$ converge to $x_\circ \in \overline{D\phi}$ as $n \rightarrow \infty$. If there exists a solution $x^n(t)$ to the evolution variational inequality (71) with respect to ϕ_n with initial condition x_\circ^n , then there also exists a solution $x(t)$ to the evolution variational inequality with respect to ϕ with initial condition x_\circ . Moreover,*

$$x^n(t) \xrightarrow{n \rightarrow \infty} x(t), \quad \text{and} \quad \phi_n(x^n(t)) \xrightarrow{n \rightarrow \infty} \phi(x(t)) \quad \text{for all } t > 0,$$

locally uniformly on $(0, \infty)$.

6.2. Application to dislocation walls. With Theorem 4.3 established, the main task for applying Theorem 6.2 for proving evolutionary convergence is to construct a suitable metric space (X, d) , and to find minimal properties for V and W for which E_n is λ -convex for some n -independent $\lambda \in \mathbb{R}$.

We start by making the state space of (7) precise. We consider any

$$x^n \in \Omega_n := \{0 \leq x_1 \leq x_2 \leq \dots \leq x_n \leq 1\} \quad \text{and} \quad b^n \in \{-1, 1\}^n, \quad (72)$$

and switch to the equivalent description in terms of $x_n^{\pm} \in \Omega_n^{\pm}$ (defined in (1)) or the empirical measures μ_n^{\pm} or μ_n whenever convenient. Note that Ω_n allows for particles of the same type to be at the same position, while (7) is ill-defined at such states. However, we consider instead the evolution variational inequality of E_n , which allows for such x^n . Moreover, we prove in (76) that any solution to (7) satisfies the evolution variational inequality of E_n .

A technical difficulty for choosing (X, d) is that X and d are not allowed to depend on n in Theorem 6.2. While the gradient flow (7) conserves the mass of positive particles n^+/n , this value can vary for different values of n . We account for both effects by allowing the mass of positive particles to vary in X , and to include the confinement to fixed mass in the energy.

With these considerations, we choose the space $X = M([0, 1])$. Setting for $\mu, \nu \in M([0, 1])$ the masses $\sigma^{\pm} := \mu^{\pm}([0, 1])$ and $\iota^{\pm} := \nu^{\pm}([0, 1])$, we equip $M([0, 1])$ with the following adjusted Wasserstein distance:

$$\mathbf{W}^2(\mu, \nu) := (\sigma^+ \wedge \iota^+) W^2\left(\frac{\mu^+}{\sigma^+}, \frac{\nu^+}{\iota^+}\right) + |\sigma^+ - \iota^+| + (\sigma^- \wedge \iota^-) W^2\left(\frac{\mu^-}{\sigma^-}, \frac{\nu^-}{\iota^-}\right) + |\sigma^- - \iota^-|, \quad (73)$$

where W denotes the 2-Wasserstein distance in $\mathcal{P}([0, 1])$, and $\sigma^+, \iota^+ \in (0, 1)$. We motivate the prefactor of $|\sigma^{\pm} - \iota^{\pm}|$ by

$$1 = \max_{\mu, \nu \in \mathcal{P}([0, 1])} W^2(\mu, \nu).$$

Since W is bounded, the case $\sigma^+ = 0$ (i.e. $\mu^+ = 0$ and $\mu^- \in \mathcal{P}([0, 1])$) is easily dealt with by setting

$$\mathbf{W}^2(\mu, \nu) := \iota^+ + \iota^- W^2\left(\mu^-, \frac{\nu^-}{\iota^-}\right) + |1 - \iota^-|. \quad (74)$$

By the symmetry in the expression of \mathbf{W} , we treat the cases $\sigma^- = 0$, $\iota^+ = 0$ or $\iota^- = 0$ similarly.

We note that on the closed subspace

$$M_{\sigma^+}([0, 1]) := \{\mu \in M([0, 1]) : \mu^+([0, 1]) = \sigma^+\}, \quad \text{for some } 0 < \sigma^+ < 1,$$

the expression for \mathbf{W} simplifies to

$$\mathbf{W}^2(\mu, \nu) := \sigma^+ W^2\left(\frac{\mu^+}{\sigma^+}, \frac{\nu^+}{\sigma^+}\right) + \sigma^- W^2\left(\frac{\mu^-}{\sigma^-}, \frac{\nu^-}{\sigma^-}\right). \quad (75)$$

For $\sigma^+ \in \{0, 1\}$, we identify $M_{\sigma^+}([0, 1])$ as $\mathcal{P}([0, 1])$ equipped with W .

Lemma 6.3 lists the required properties of the space $(M([0, 1]), \mathbf{W})$. A proof is given in Appendix B.

Lemma 6.3 (properties of $(M([0, 1]), \mathbf{W})$). *$(M([0, 1]), \mathbf{W})$ is a complete, separable, sequentially compact metric space. The closed subspace $M_{\sigma^+}([0, 1])$ is, in addition, non-positively curved for any $0 \leq \sigma^+ \leq 1$. Moreover,*

- (i) $\mathbf{W}((\mu^+, \mu^-), (\nu^+, \nu^-)) = \mathbf{W}((\mu^-, \mu^+), (\nu^-, \nu^+))$;
- (ii) for $(\mu_k) \subset M([0, 1])$, it holds that $\mu_k \rightharpoonup \mu$ if and only if $\mathbf{W}(\mu_k, \mu) \rightarrow 0$;
- (iii) let $x^n, y^n \in \Omega_n$ (defined in (72)), and $\mu_n, \nu_n \in M_{n^+/n}([0, 1])$ be the corresponding empirical measures. Then $\mathbf{W}^2(\mu_n, \nu_n) = \frac{1}{n}|x^n - y^n|^2$;
- (iv) for any endpoints $\mu_0, \mu_1 \in M_{\sigma^+}([0, 1])$, all $M([0, 1])$ -geodesics remains in $M_{\sigma^+}([0, 1])$.

We continue with λ -convexity of E_n on Ω_n . We note that on \mathbb{R}^d , $f: \mathbb{R}^d \rightarrow \mathbb{R}$ is λ -convex if

$$x \mapsto f(x) - \frac{\lambda}{2}|x|^2 \quad \text{is convex on } \mathbb{R}^d.$$

The following result shows how λ -convexity of E_n follows from $\tilde{\lambda}$ -convexity of V and W :

Proposition 6.4 (λ -convexity of E_n on Ω_n). *Let V be $\tilde{\lambda}$ -convex on $(0, \infty)$ and W be $\tilde{\lambda}$ -convex on \mathbb{R} with $\tilde{\lambda} \leq 0$. Then E_n is $\tilde{\lambda}_n$ -convex on Ω_n , with $\tilde{\lambda}_n := -2\alpha_n^3 \frac{1}{n} \tilde{\lambda}$.*

Proof. By convexity of $V(x) - \frac{1}{2}\tilde{\lambda}x^2$ and $W(x) - \frac{1}{2}\tilde{\lambda}x^2$, it follows that

$$x^n \mapsto E_n(x^n) + \frac{\tilde{\lambda}}{2} \left(\sum_{p=\pm} \frac{1}{n^2} \sum_{i=1}^{n^p} \sum_{j=1}^{i-1} \alpha_n (\alpha_n (x_i^p - x_j^p))^2 + \frac{1}{n^2} \sum_{i=1}^{n^+} \sum_{j=1}^{n^-} \alpha_n (\alpha_n (x_i^+ - x_j^-))^2 \right)$$

is convex on Ω_n . It remains to compute the eigenvalues of the Hessian of the term in parentheses. Observing that

$$\sum_{p=\pm} \frac{1}{n^2} \sum_{i=1}^{n^p} \sum_{j=1}^{i-1} \alpha_n (\alpha_n (x_i^p - x_j^p))^2 + \frac{1}{n^2} \sum_{i=1}^{n^+} \sum_{j=1}^{n^-} \alpha_n (\alpha_n (x_i^+ - x_j^-))^2 = \frac{\alpha_n^3}{2n^2} \sum_{i=1}^n \sum_{j=1}^n (x_i - x_j)^2,$$

we obtain that the Hessian is given by

$$\frac{2\alpha_n^3}{n^2} (nI - \mathbf{1} \otimes \mathbf{1}),$$

where $\mathbf{1} = (1, \dots, 1)^T \in \mathbb{R}^n$. Hence, the eigenvalues of the Hessian are $2\alpha_n^3 \frac{1}{n}$ and 0. We conclude that $x^n \mapsto E_n(x^n) + \alpha_n^3 \frac{1}{n} \tilde{\lambda} |x^n|^2$ is convex on Ω_n , and thus E_n is $-2\alpha_n^3 \frac{1}{n} \tilde{\lambda}$ -convex on Ω_n . \square

We note that if V is $(\tilde{\lambda} + b)$ -convex with $b > 0$, then $\tilde{\lambda}_n$ in Proposition 6.4 need not increase, as the interaction term in E_n corresponding to the positive particles is invariant under translation of the positive particles. A similar invariance holds for the negative particles.

Adding $\tilde{\lambda}$ -convexity to Assumption 4.1, we obtain

Assumption 6.5 (Properties of V and W for dynamics). *There exists a $\tilde{\lambda} \in \mathbb{R}$ such that V and W satisfy*

- (i) $V \in L_{\text{loc}}^1(\mathbb{R})$ is even, and $\tilde{\lambda}$ -convex on $(0, \infty)$;
- (ii) $W: \mathbb{R} \rightarrow \mathbb{R}$ is even and $\tilde{\lambda}$ -convex on \mathbb{R} .

Next we show that for solutions $x^n(t)$ of (7) (if they exist), the corresponding curve $\mu_n(t)$ satisfies an evolution variational inequality. By $\tilde{\lambda}_n$ -convexity on Ω_n ,

$$E_n(y^n) \geq E_n(x^n) + (y^n - x^n) \cdot \nabla E_n(x^n) + \frac{1}{2} \tilde{\lambda}_n |x^n - y^n|^2 \quad \text{for all } x^n, y^n \in \Omega_n,$$

and thus, for any solution $x^n(t)$ of (7) and any $y^n \in \Omega_n$, we find

$$\begin{aligned} \frac{1}{2n} \frac{d}{dt} |x^n - y^n|^2 &= \frac{1}{n} (x^n - y^n) \cdot \frac{dx^n}{dt} = (y^n - x^n) \cdot \nabla E_n(x^n) \\ &\leq E_n(y^n) - E_n(x^n) - \frac{1}{2} \tilde{\lambda}_n |x^n - y^n|^2, \end{aligned} \quad (76)$$

which is of the form (71). Using Lemma 6.3.(iii), we write (76) in terms of the corresponding empirical measures $\mu_n(t), \nu_n \in M_{n^+/n}([0, 1])$. Observing that $E_n(\nu)$ equals ∞ if ν is not an empirical measure as in (115), we find from (76) that

$$\frac{1}{2} \frac{d}{dt} \mathbf{W}^2(\mu_n(t), \nu) + \alpha_n^3 \tilde{\lambda} \mathbf{W}^2(\mu_n(t), \nu) + E_n(\mu_n(t)) \leq E_n(\nu),$$

for a.e. $t > 0$ and all $\nu \in M_{n^+/n}([0, 1])$. (77)

Below, in Theorem 6.7, we prove that (77) has a unique solution for any $\mu_n^\circ \in M_{n^+/n}([0, 1])$, while existence and uniqueness of solutions to (7) is not clear for all such initial data. Hence, we prefer to work with (77) instead of (7).

Next we show how $\tilde{\lambda}_n$ -convexity of E_n on Ω_n implies λ_n -convexity of E_n on $M_{n^+/n}([0, 1])$.

Proposition 6.6 (λ -convexity of E_n and E on $M_{\sigma^+}([0, 1])$). *Let V, W satisfy Assumption 6.5 and $\alpha_n \rightarrow \alpha > 0$. Then, setting*

$$\lambda_n := -2\alpha_n^3 \tilde{\lambda} \quad \text{and} \quad \lambda := -2\alpha^3 \tilde{\lambda},$$

E_n is λ_n -convex on $M_{n^+/n}([0, 1])$ for all n large enough and all $n^+ \in \{0, \dots, n\}$, and E is λ -convex on $M_{\sigma^+}([0, 1])$ for all $0 \leq \sigma^+ \leq 1$.

Proof. Proposition 6.4 implies that $x \mapsto E_n(x) + \alpha_n^3 \tilde{\lambda}_n |x - y|^2$ is convex for any $y \in \Omega_n$. Hence,

$$\mu_n \mapsto E_n(\mu_n) + \alpha_n^3 \tilde{\lambda} \mathbf{W}^2(\mu_n, \nu_n)$$

is convex in $M_{n^+/n}([0, 1])$ along geodesics, where μ_n, ν_n are empirical measures corresponding to elements of Ω_n . Since Γ -convergence conserves convexity, we obtain from Lemma 6.3.(ii) that

$$\mu \mapsto E(\mu) + \alpha^3 \tilde{\lambda} \mathbf{W}^2(\mu, \nu)$$

is convex in $M_{\sigma^+}([0, 1])$ along geodesics for any $0 \leq \sigma^+ \leq 1$ and any $\nu \in M_{\sigma^+}([0, 1])$. Hence, E is λ -convex in $M_{\sigma^+}([0, 1])$. \square

Theorem 6.7 (Evolutionary convergence in the case $\alpha_n \rightarrow \alpha > 0$). *Let V, W satisfy Assumption 6.5. Then for any sequence $x_n^\circ \in \Omega_n$ for which the corresponding sequence of empirical measure $\mu_n^\circ \in M_{n^+/n}([0, 1])$ converges narrowly to some μ° , it holds that (77) attains a unique solution $\mu_n(t)$ with initial condition μ_n° for all $n \in \mathbb{N}$. Moreover,*

$$\mu_n(t) \xrightarrow{n \rightarrow \infty} \mu(t), \quad \text{and} \quad E_n(\mu_n(t)) \xrightarrow{n \rightarrow \infty} E(\mu(t)) \quad \text{for all } t > 0,$$

locally uniformly on $(0, \infty)$, where $\mu(t)$ is the unique solution to

$$\frac{1}{2} \frac{d}{dt} \mathbf{W}^2(\mu(t), \nu) + \alpha^3 \tilde{\lambda} \mathbf{W}^2(\mu(t), \nu) + E(\mu(t)) \leq E(\nu),$$

for a.e. $t > 0$ and all $\nu \in M_{\sigma^+}([0, 1])$, (78)

with initial condition μ° , and $\sigma^+ := \mu^{\circ,+}([0, 1])$.

Proof. We first prove existence and uniqueness of the solution to (77) with initial condition μ_n° by showing that Theorem 6.1 applies. Lemma 6.3 implies that the space $(M_{n^+/n}([0, 1]), \mathbf{W})$ satisfies the conditions of Theorem 6.1, and Proposition 6.6 guarantees the required λ_n -convexity of E_n . Since $D(E_n)$ is finite whenever all particles are at different positions, it holds that $\mu_n^\circ \in \overline{D(E_n)}$. Hence, Theorem 6.1 guarantees that (77) attains a unique solution $\mu_n(t)$ with initial condition μ_n° .

Similarly, we prove existence and uniqueness of the solution to (78) with initial condition μ° . Again, Lemma 6.3 implies that the space $(M_{\sigma^+}([0, 1]), \mathbf{W})$ satisfies the conditions of Theorem 6.1, and Proposition 6.6 guarantees the required λ -convexity of E . Since

$$D(E) \supset \{\mu \in M_{\sigma^+}([0, 1]) : \mu^\pm \in L^\infty(0, 1)\}$$

it holds that $\overline{D(E)} = M_{\sigma^+}([0, 1]) \ni \mu^\circ$. Hence, Theorem 6.1 guarantees that (78) attains a unique solution $\mu(t)$ with initial condition μ° .

Next we prepare for applying Theorem 6.2. First, we rewrite the evolution variational inequalities (77) and (78) in terms of the n -independent space $(M([0, 1]), \mathbf{W})$, which, by Lemma 6.3, satisfies the condition of Theorem 6.2. To this aim, we set

$$\phi_n(\boldsymbol{\mu}) := E_n(\boldsymbol{\mu}) + \chi_{\{\mu^+ = n^+/n\}} \quad \text{and} \quad \phi(\boldsymbol{\mu}) := E(\boldsymbol{\mu}) + \chi_{\{\mu^+ = \sigma^+\}},$$

where the characteristic function is given by

$$\chi_A := \begin{cases} 0 & \text{if } A \text{ holds,} \\ \infty & \text{otherwise.} \end{cases}$$

It is obvious that $\boldsymbol{\mu}_n(t)$ satisfies

$$\frac{1}{2} \frac{d}{dt} \mathbf{W}^2(\boldsymbol{\mu}_n(t), \boldsymbol{\nu}) + \alpha_n^3 \tilde{\lambda} \mathbf{W}^2(\boldsymbol{\mu}_n(t), \boldsymbol{\nu}) + \phi_n(\boldsymbol{\mu}_n(t)) \leq \phi_n(\boldsymbol{\nu}), \quad \text{for a.e. } t > 0 \text{ and all } \boldsymbol{\nu} \in M([0, 1]). \quad (79)$$

However, $(M([0, 1]), \mathbf{W})$ may not satisfy the conditions of Theorem 6.1, and thus we use a different argument to show that (79) has a unique solution. Let $\tilde{\boldsymbol{\mu}}_n \in AC_{\text{loc}}(0, \infty; M([0, 1]))$ satisfy (79) with initial condition $\boldsymbol{\mu}_n^\circ$. Then $\phi_n(\tilde{\boldsymbol{\mu}}_n(t)) < \infty$ for any $t > 0$, and thus $\tilde{\boldsymbol{\mu}}_n(t) \in M_{n^+/n}([0, 1])$ for a.e. $t > 0$. Hence, $\tilde{\boldsymbol{\mu}}_n$ is a solution to (77). Since (77) has a unique solution, $\tilde{\boldsymbol{\mu}}_n = \boldsymbol{\mu}_n$. An analogous argument show that $\boldsymbol{\mu}(t)$ satisfies

$$\frac{1}{2} \frac{d}{dt} \mathbf{W}^2(\boldsymbol{\mu}, \boldsymbol{\nu}) + \alpha^3 \tilde{\lambda} \mathbf{W}^2(\boldsymbol{\mu}, \boldsymbol{\nu}) + \phi(\boldsymbol{\mu}) \leq \phi(\boldsymbol{\nu}), \quad \text{for all } t > 0, \boldsymbol{\nu} \in M([0, 1]), \quad (80)$$

and that (80) has no other solution in $AC_{\text{loc}}(0, \infty; M([0, 1]))$ with initial condition $\boldsymbol{\mu}^\circ$.

Second, we choose $\lambda - 1$ as the convexity constant. Then, for all n large enough, $\lambda_n \geq \lambda - 1$. Since the existence and uniqueness of solutions to the evolution variational inequality are invariant under lowering the value of λ , (79) and (80) still have $\boldsymbol{\mu}_n$ and $\boldsymbol{\mu}$ respectively as their unique solutions when we replace λ_n and λ by $\lambda - 1$.

Third, by Lemma 6.3.(iv) and

$$\overline{D(\phi_n)} = M_{n^+/n}([0, 1]) \quad \text{and} \quad \overline{D(\phi)} = M_{\sigma^+}([0, 1]),$$

$(\lambda - 1)$ -convexity of ϕ_n and ϕ is implied by the λ_n - and λ -convexity of E_n and E .

Fourth, we prove Γ -convergence of ϕ_n to ϕ in the narrow topology. To establish the liminf-inequality (17a), it is enough to consider sequences $\boldsymbol{\nu}_n$ for which $\phi_n(\boldsymbol{\nu}_n)$ is uniformly bounded. Then, $\boldsymbol{\nu}_n^+([0, 1]) = \frac{1}{n}n^+ \rightarrow \sigma$ as $n \rightarrow \infty$, and thus

$$\liminf_{n \rightarrow \infty} \phi_n(\boldsymbol{\nu}_n) \geq \liminf_{n \rightarrow \infty} E_n(\boldsymbol{\nu}_n) \geq E(\boldsymbol{\nu}) = \phi(\boldsymbol{\nu}).$$

The limsup-inequality (17b) follows from Theorem 4.3 by taking a recovery sequence for E_n which satisfies $\mu_n^+([0, 1]) = \frac{1}{n}n^+$. Then

$$\limsup_{n \rightarrow \infty} \phi_n(\boldsymbol{\nu}_n) = \limsup_{n \rightarrow \infty} E_n(\boldsymbol{\nu}_n) \leq E(\boldsymbol{\nu}) \leq \phi(\boldsymbol{\nu}).$$

Taking all four conditions into account, Theorem 6.2 applies to the solutions of (79) and (80) with λ_n and λ replaced by $\lambda - 1$. Since these solutions are unique and given by $\boldsymbol{\mu}_n$ and $\boldsymbol{\mu}$, the prove of the convergence statements in Theorem 6.7 is complete. \square

While Theorem 6.7 gives a unique characterisation of the limiting curve

$$\boldsymbol{\mu} \in AC_{\text{loc}}(0, \infty; M_{\sigma^+}([0, 1])),$$

it does not provide us with an explicit PDE which $\boldsymbol{\mu}$ satisfies. Next, we characterise this PDE informally. Nonetheless, the derivation is rigorous for limited choices of V and W , which include the setting of dislocation walls in §2.

Let us set $\alpha_n = \alpha = 1$ for convenience. We rewrite (7) as

$$\frac{d}{dt} x_i^\pm = -(V' * \mu_n^\pm)(x_i^\pm) - (W' * \mu_n^\mp)(x_i^\pm) \mp \gamma_n^2, \quad i = 1, \dots, n^\pm,$$

where we define $V'(0) := 0$. Given $\varphi^\pm \in C_c^\infty((0, \infty) \times (0, 1))$, we compute from

$$0 = \frac{1}{n} \sum_{i=1}^{n^\pm} \int_0^T \frac{d}{dt} \varphi^\pm(t, x_i^\pm(t)) dt$$

with Schochet's symmetrisation argument [Sch96] that μ_n satisfies

$$0 = \sum_{p=\pm} \left[\int_0^\infty \int_0^1 \frac{\partial \varphi^p}{\partial t} d\mu_n^p dt - \int_0^\infty \left(\iint_{[0,1]^2} V'(x-y) \frac{(\varphi^p)'(x) - (\varphi^p)'(y)}{2} d(\mu_n^p \otimes \mu_n^p)(x, y) \right. \right. \\ \left. \left. + \iint_{[0,1]^2} W'(x-y) (\varphi^p)'(x) d(\mu_n^p \otimes \mu_n^{-p})(x, y) + p\gamma_n^2 \int_0^1 (\varphi^p)'(x) d\mu_n^p(x) \right) dt \right], \quad (81)$$

where $(\varphi^p)'$ denotes the spatial derivative. Assuming that $xV'(x)$ is bounded on $[-1, 1]$ and continuous on $[-1, 1] \setminus \{0\}$, and $W' \in C_b([-1, 1])$, we can pass to the limit $n \rightarrow \infty$ in (81) to obtain

$$0 = \sum_{p=\pm} \left[\int_0^\infty \int_0^1 \frac{\partial \varphi^p}{\partial t} d\mu^p dt - \int_0^\infty \left(\iint_{[0,1]^2} V'(x-y) \frac{(\varphi^p)'(x) - (\varphi^p)'(y)}{2} d(\mu^p \otimes \mu^p)(x, y) \right. \right. \\ \left. \left. + \iint_{[0,1]^2} W'(x-y) (\varphi^p)'(x) d(\mu^p \otimes \mu^{-p})(x, y) + p\gamma^2 \int_0^1 (\varphi^p)'(x) d\mu^p(x) \right) dt \right], \quad (82)$$

which is commonly abbreviated by (8).

7. EXAMPLE OF NON-CONVERGENCE IN THE CASE $\frac{1}{n}\alpha_n \rightarrow \alpha$

While Γ -convergence implies convergence of global minima of E_n to a global minimum of E , it does not imply convergence of local minima of E_n to a local minimum of E . In this section, we show that the setting of dislocation walls exhibits such an example where local minima do not converge to an extremal point of E . Moreover, this example is physically meaningful [DPG15], and adds to other known examples which show that dislocation networks cannot be fully characterised in terms of the dislocation density alone.

We start from the numerical case studies in [DPG15, Fig. 5,6,7]. It considers the gradient flow of E_n given by (7) with V as in (11) and W_1 as in (12). The parameters are $n^+ = n^-$, $\gamma_n = 0$ and $\alpha_n = C\sqrt{n}$ for some fixed $C > 0$. The initial state is fully separated (9). The question in this case study is whether the long-time behaviour exhibits mixing. The conclusion from the numerical computations is that for small values of n , full separation is conserved in time, while for large values of n , mixing occurs (i.e., $\mathcal{O}(n^2)$ couples (x_i^+, x_j^-) swap position). Mixing is also observed in [DPG15] in their postulated \mathbf{W} -gradient flow of E given by

$$\partial_t \rho^\pm = \left[\int_{\mathbb{R}} V \right] (\rho^\pm (\rho^\pm)')' + \left[\int_{\mathbb{R}} W \right] (\rho^\pm (\rho^\mp)')'. \quad (83)$$

We call (83) “the \mathbf{W} -gradient flow of E ” because it is given by the formal formula (see [AGS08, (11.1.6)]) given by

$$\partial_t \rho^\pm = \operatorname{div} \left(\rho^\pm \nabla \frac{\delta E(\rho)}{\delta \rho^\pm} \right),$$

where $\delta/\delta \rho^\pm$ denotes the L^2 -gradient of E .

7.1. Numerical observations. We extend the aforementioned case study in [DPG15] by varying α_n . We set $n^+ = n^-$, $\gamma_n = 0$, and take the equispaced initial condition

$$x_{\circ, i}^+ = \frac{i-1}{n}, \quad x_{\circ, i}^- = \frac{1}{2} + \frac{i}{n}, \quad i = 1, \dots, n^+, \quad (84)$$

which is fully separated (9). Figure 5 shows the gradient flow trajectories for $n = 2^6$. These trajectories are computed with the ‘ode15s’ solver [SR97] in MATLAB, which is designed for

stiff systems and has variable time steps. The variable time steps allow to compute the long-time behaviour of $x^n(t)$ (we take $T = 10^{10}$ as the end time) without significantly increasing the computation time.

For large values of t , we observe from Figure 5 that the case $\alpha_n = 2n$ exhibits full separation. Moreover, the particles seem to spread out evenly, which corresponds to the continuum state $\rho_{\text{sep}} = (\mathcal{L}_{(0,1/2)}, \mathcal{L}_{(1/2,1)})$ as defined in (10).

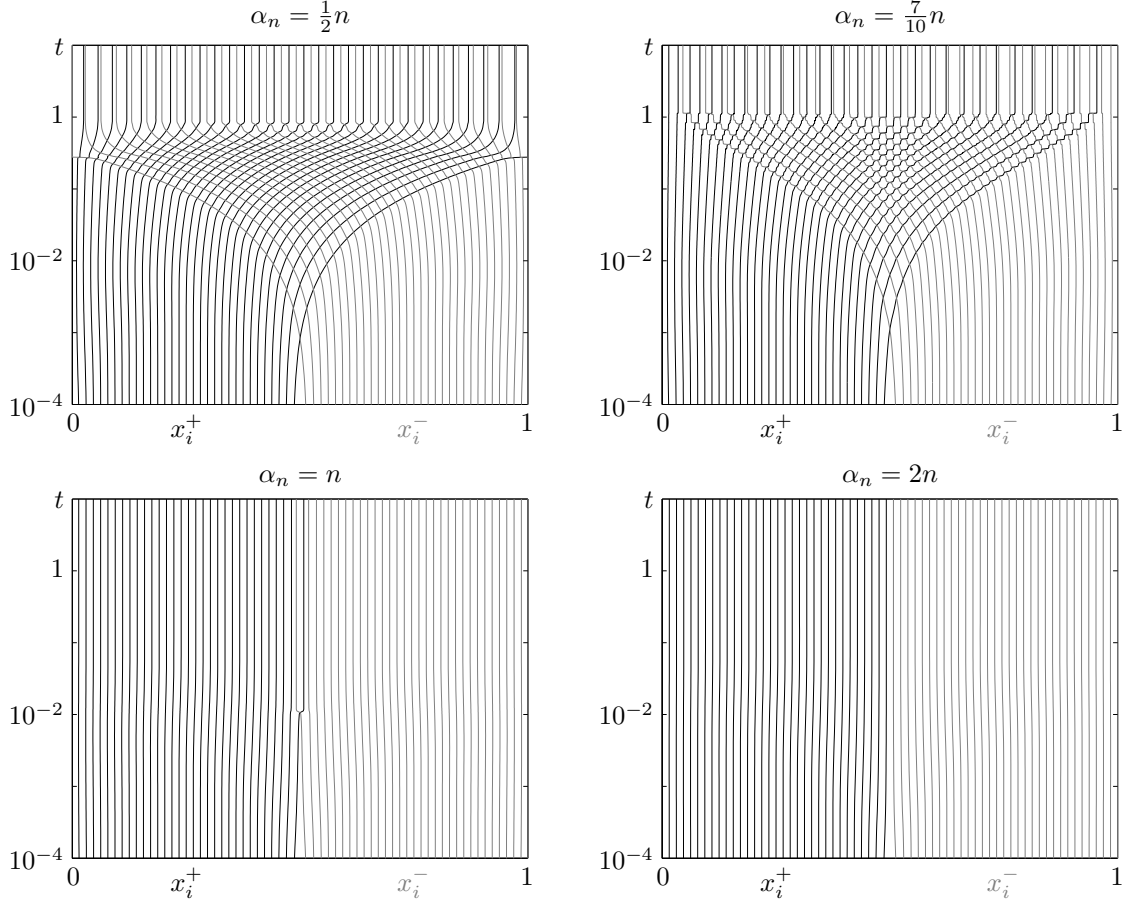


FIGURE 5. Trajectories of the solutions $x_i^\pm(t)$ to the gradient flow (7) with $n = 2^6$ and initial condition given by (84). For increasing values of α_n , less particles swap position as time passes. For $t > 10$ there is no visible time dependence on the trajectories.

On the other end of the spectrum, the case $\alpha_n = \frac{1}{2}n$ exhibits complete mixing at $t = T$, i.e.,

$$0 = x_1^+ \leq x_1^- < x_2^+ < x_2^- < x_3^+ < \dots < x_{n-1}^- < x_{n+}^+ \leq x_{n-}^- = 1. \quad (85)$$

Moreover, the particles seem to spread out evenly, which corresponds to the continuum state

$$\rho_{\text{mix}} = \left(\frac{1}{2}\mathcal{L}_{(0,1)}, \frac{1}{2}\mathcal{L}_{(0,1)}\right).$$

In the intermediate case $\alpha_n = n$, only the middle two particles swap position. The profile at $t = T$ still corresponds to the continuum state ρ_{sep} . When $\alpha_n = \frac{7}{10}n$, many particles swap positions, but not all, and thus (85) is not satisfied at $t = T$. Indeed, the average number of positive particles near the left barrier exceeds the average number of negative particles, which corresponds to a different continuum state than ρ_{mix} .

Next we focus on the case $\alpha_n = 2n$ at $t = T$, and check numerically whether full separation (9) occurs for several values of n . To this aim, we compute

$$d_n^{+-} := \alpha_n(x_1^- - x_{n+}^+) \quad \text{and} \quad \mathbf{W}(\boldsymbol{\mu}_n, \boldsymbol{\rho}_{\text{sep}}). \quad (86)$$

Table 5 shows that $d_n^{+-} > 0$. Since the logarithmic singularity of V keeps particles of the same type ordered, we conclude full separation for all values of n in Table 5. Moreover, to test whether $\mathbf{W}(\boldsymbol{\mu}_n, \boldsymbol{\rho}_{\text{sep}}) \rightarrow 0$ as $n \rightarrow \infty$, we compute the decay rate q in $\mathbf{W}(\boldsymbol{\mu}_n, \boldsymbol{\rho}_{\text{sep}}) \sim Cn^{-q}$ by

$$q_n = \frac{\log(\mathbf{W}(\boldsymbol{\mu}_n, \boldsymbol{\rho}_{\text{sep}})) - \log(\mathbf{W}(\boldsymbol{\mu}_{2n}, \boldsymbol{\rho}_{\text{sep}}))}{\log 2}. \quad (87)$$

Table 5 shows that $q_n \approx 1$. Consequently, we expect that $\boldsymbol{\mu}_n \rightarrow \boldsymbol{\rho}_{\text{sep}}$ as $n \rightarrow \infty$. We discuss the meaning of the values of \bar{d}_n^{\pm} after proving in §7.2 that for $\alpha_n = \alpha n$ with α large enough, E_n attains a fully separated local minimiser for all n .

n	d_n^{+-}	q_n	\bar{d}_n^{\pm}
2^4	2.102	1.022	1.069
2^5	2.026	1.010	1.033
2^6	1.989	1.005	1.017
2^7	1.971	1.002	1.008
2^8	1.962	1.001	1.004
2^9	1.959	1.000	1.002
2^{10}	1.955	1.001	1.001
2^{11}	1.954	1.001	1.001
2^{12}	1.953	—	1.000

TABLE 5. Values computed from (86), (87) and (98) for $x^n(T)$, which is the solution at $t = T$ of the gradient flow (7) with $\alpha_n = 2n$ and initial condition (84). $d_n^{+-} > 1.9$ means that $x^n(T)$ is fully separated (9), $q_n \approx 1$ suggests that $\mathbf{W}(\boldsymbol{\mu}_n(T), \boldsymbol{\rho}_{\text{sep}}) \leq C\frac{1}{n}$, and $\bar{d}_n^{\pm} \geq 1$ means that neighbouring particles of the same type are separated by a distance of at least $\frac{1}{n}$ if they are located in the interval $(\frac{1}{4}, \frac{3}{4})$.

We repeat similar simulations for $t = T$, $\alpha_n = \frac{1}{2}n$ and $n = 2^4, 2^5, \dots, 2^9$ to inspect whether complete mixing (85) depends on n . The reason for the relatively small values of n is that during a swapping event of two particles, the force acting on both particles is of the order of n , which requires a small time step to resolve. Moreover, from Figure 5 we expect $\mathcal{O}(n^2)$ such swapping events to occur.

For all experiments in Table 6 (including $n = 2^9$) we have verified that x^n is completely mixed (85). Moreover, similar to (87), we compute

$$\tilde{q}_n = \frac{\log(\mathbf{W}(\boldsymbol{\mu}_n, \boldsymbol{\rho}_{\text{mix}})) - \log(\mathbf{W}(\boldsymbol{\mu}_{2n}, \boldsymbol{\rho}_{\text{mix}}))}{\log 2}, \quad (88)$$

and speculate from Table 6 that $\boldsymbol{\mu}_n \rightarrow \boldsymbol{\rho}_{\text{mix}}$ as $n \rightarrow \infty$. However, the values for n remain relatively small, and we have not found a theoretical lower bound on α such that complete mixing occurs for $\alpha_n = \alpha n$ for all n large enough.

To get insight in the macroscopic dynamics leading to the completely mixed state, we illustrate in Figure 6 a few time slices of the piecewise-constant discrete density $\rho_n^{\pm}(t, x)$ given by

$$\rho_n^{\pm}(t, x) := \frac{1}{n(x_{i+1}^{\pm}(t) - x_i^{\pm}(t))}, \quad \text{with } i \text{ such that } x_i^{\pm}(t) < x \leq x_{i+1}^{\pm}(t).$$

The plots in Figure 6 are the linear interpolations of ρ_n^{\pm} evaluated at the midpoints, i.e.,

$$(m_i^{\pm}(t), \rho_n^{\pm}(t, m_i^{\pm}(t)))_{i=1}^{n^{\pm}-1}, \quad \text{where } m_i^{\pm}(t) := \frac{1}{2}(x_{i+1}^{\pm}(t) + x_i^{\pm}(t)). \quad (89)$$

n	\tilde{q}_n
2^4	0.940
2^5	0.944
2^6	0.965
2^7	0.981
2^8	0.990

TABLE 6. Similar to Table 5, but here with $\alpha_n = \frac{1}{2}n$ and \tilde{q}_n as in (88). $\tilde{q}_n \approx 1$ suggests that $\mu_n(T)$ converges to ρ_{mix} as $n \rightarrow \infty$.

We observe that $(\rho_n^+ + \rho_n^-)(t)$ is not constant as a function of x during the evolution, while $(\rho_n^+ + \rho_n^-)(0)$ and $(\rho_n^+ + \rho_n^-)(T)$ appear to be constant in x . This is in line with a locally mixed state having lower energy than a locally separated state (because of $V > W$), which allows for a denser packing of particles (as V and W are decreasing on $(0, \infty)$). Moreover, the spatial change from local separation to mixing is characterised by a spatial jump-discontinuity in $\rho_n^\pm(t)$. Figure 5 suggests that the location of this ‘shock’ propagates in time to the boundary, which it meets at some $t \in (\frac{1}{10}, \frac{1}{3})$. We expect the wiggles in the profiles of $\rho_n^\pm(t)$ close to the shock to be caused by frustration due to the difference in the local density of the positive and negative particles. Finally, we observe small boundary-layer effects close to the barriers at $x \in \{0, 1\}$. We do not study these effects here, and refer to [HHvM16] for analysis and numerics of such boundary layers at equilibrium.

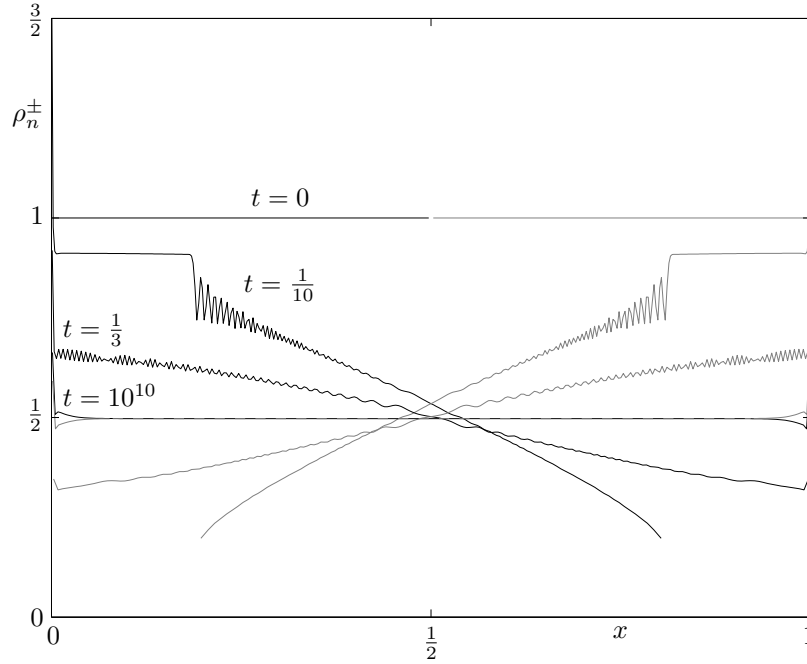


FIGURE 6. Several time slices of the discrete density ρ_n^+ (black) and ρ_n^- (gray) (see (89)) to the gradient flow (7) with $n = 2^9$, $\alpha_n = \frac{1}{2}n$, and initial condition given by (84). The profiles of $\rho_n^\pm(t)$ show typical stages of the evolution from ρ_{sep} to ρ_{mix} on the discrete level.

7.2. Local minima for $\alpha_n = \alpha n$ with α large. Proposition 1.2 gives a quantitative upper bound on the asymptotic behaviour of α_n for which E_n has a local minimum which is fully separated.

For the sake of its proof and later use, we set

$$r^* := \arg \max_{(0, \infty)} |W'(r)|. \quad (90)$$

We also rely on the following property of V , which we prove in Appendix A:

$$\forall C > 0 \exists \alpha_0 > 0 : \sup_{\alpha > \alpha_0} [CV_{\text{eff}}(\alpha/C) - V(\alpha x)] > 0 \implies x \geq \frac{1}{4C}. \quad (91)$$

Proof of Proposition 1.2. For any $n^\pm \geq 2$ and $\alpha > r^*/n$, we define the open, convex set

$$\Omega_n^* := \{(x^{n,+}, x^{n,-}) \in \Omega_n^+ \times \Omega_n^- : x_1^+ = 0, x_{n-}^- = 1, d_n^{+-} > r^*\},$$

where Ω_n^\pm , d_n^{+-} and r^* are defined in (1), (86) and (90) respectively. Since $\alpha > r^*/n$, Ω_n^* is not empty. We further note that all elements of Ω_n^* satisfy the full separation condition (9). We also observe that in the expression for $E_n(x^n)$ as in (2), the argument of W remains smaller than $-r^*$ for all $x^n \in \Omega_n^*$. Since W is strictly convex on $(-\infty, -r^*)$, and V is strictly convex on $(0, \infty)$, we conclude that E_n is strictly convex on Ω_n^* . Hence, E_n has a unique minimiser in $\overline{\Omega_n^*}$, which we set as \bar{x}^n . It remains to prove that $\bar{x}^n \in \Omega_n^*$, which by the strict convexity of E_n on Ω_n^* implies that \bar{x}^n is a local minimiser of E_n on the full state space $\Omega_n^+ \times \Omega_n^-$.

We need several *a priori* estimates on \bar{x}^n to prove that $\bar{x}^n \in \Omega_n^*$. We start by showing that we can add an extra negative particle ‘inside’ $\bar{x}^{n,-}$ without increasing the total energy by too much, i.e.,

$$\exists C > 0, \alpha_0 > \frac{1}{2}r^* \forall n^\pm \geq 2, \alpha > \alpha_0 \exists z \in (\bar{x}_1^-, \bar{x}_{n-}^-) : \quad \frac{\alpha}{n} \left[\sum_{j=1}^{n^+} W(\alpha n(z - \bar{x}_j^+)) + \sum_{j=1}^{n^-} V(\alpha n(z - \bar{x}_j^-)) \right] \leq \frac{C}{n} \alpha V_{\text{eff}}\left(\frac{\alpha}{C}\right). \quad (92)$$

The restriction to negative particles is not restrictive because of the symmetry of E_n (see (19)). To prove (92), we take $n^\pm \geq 2$ and $\alpha > \alpha_0$ arbitrary. We choose z as one of the midpoints of $\bar{x}^{n,-}$, which we select by a similar argument as in Step 2 of the proof of Lemma 4.10.(vii). On the one hand, the argument is easier since we only add one particle, but on the other hand, we need uniformity of C with respect to α . The sum in (92) corresponds to Σ_2 in (37). We construct the index sets J_1^- and J_2^- in a similar fashion. To establish estimates corresponding to those in (39) and (40), we set d_*^- as in (38). Since $\alpha_0 > \frac{1}{2}r^*$, we obtain $x_o^n \in \Omega_n^*$ (see (84)). We estimate

$$\frac{\alpha}{5} V(\alpha n d_*^-) < E_n(\bar{x}^n) \leq E_n(x_o^n) < \frac{\alpha}{n} \sum_{i=1}^n \sum_{j=1}^{i-1} V(\alpha n(x_{o,i} - x_{o,j})) < \alpha \sum_{i=1}^n V(\alpha i) < \alpha V_{\text{eff}}(\alpha). \quad (93)$$

Applying (91) with $C = 5$ and taking α_0 accordingly, we conclude that

$$n d_*^- \geq \frac{1}{20}, \quad (94)$$

and construct the index set J_1^- as in (42) with respect to this estimate. Regarding the index set J_2^- , we obtain from (93) that the corresponding property of (43) reads

$$\sum_{j=1}^{n^+} W(\alpha n(\bar{x}_\ell^- - \bar{x}_j^+)) + \sum_{j=1}^{\ell-1} V(\alpha n(\bar{x}_\ell^- - \bar{x}_j^-)) + \sum_{j=\ell+2}^{\tilde{n}} V(\alpha n(\bar{x}_j^- - \bar{x}_{\ell+1}^-)) \leq 5V_{\text{eff}}(\alpha) \quad \text{for all } \ell \in J_2^-.$$

Then, choosing any $i \in J_1^- \cap J_2^-$ and setting the midpoint $z := \frac{1}{2}(\bar{x}_{i+1}^- + \bar{x}_i^-)$, we estimate

$$\begin{aligned} & \frac{\alpha}{n} \left[\sum_{j=1}^{n^+} W(\alpha n(z - \bar{x}_j^+)) + \sum_{j=1}^{n^-} V(\alpha n(z - \bar{x}_j^-)) \right] \\ & \leq \frac{\alpha}{n} \left[\sum_{j=1}^{n^+} W(\alpha n(\bar{x}_i^- - \bar{x}_j^+)) + \sum_{j=1}^{i-1} V(\alpha n(\bar{x}_i^- - \bar{x}_j^-)) \right. \\ & \quad \left. + 2V(\alpha n(\frac{1}{2}(\bar{x}_{i+1}^- - \bar{x}_i^-))) + \sum_{j=i+2}^{n^-} V(\alpha n(\bar{x}_j^- - \bar{x}_{i+1}^-)) \right] \\ & \leq \frac{\alpha}{n} (5V_{\text{eff}}(\alpha) + 2V(\alpha n \frac{1}{2} d_*^-)). \end{aligned}$$

Using (94), we continue the estimate by

$$\frac{\alpha}{n} (5V_{\text{eff}}(\alpha) + 2V(\alpha n \frac{1}{2} d_*^-)) \leq \frac{\alpha}{n} (5V_{\text{eff}}(\alpha) + 2V(\frac{1}{40}\alpha)) \leq \frac{7}{n} \alpha V_{\text{eff}}(\frac{1}{40}\alpha).$$

We conclude (92).

Using (92), we prove the following lower bound on the distance between neighbouring negative particles:

$$\exists c, \alpha_0 > 0 \forall \alpha \geq \alpha_0, n^\pm \geq 2 : \bar{d}_n^- := \min_{1 \leq i \leq n^- - 1} n(\bar{x}_{i+1}^- - \bar{x}_i^-) \geq c. \quad (95)$$

Given $\alpha \geq \alpha_0$ with α_0 as in (92) and $n^\pm \geq 2$, we derive this estimate by moving the particle \bar{x}_i^- with any index i such that

$$\bar{d}_n^- = n(\bar{x}_{i+1}^- - \bar{x}_i^-),$$

to the position z provided by (92). This yields (with abuse of notation)

$$\begin{aligned} 0 & \leq E_n(\bar{x}^{n,+}, (\bar{x}_1^-, \dots, \bar{x}_{i-1}^-, z, \bar{x}_{i+1}^-, \dots, \bar{x}_{n^-}^-)^T) - E_n(\bar{x}^n) \\ & = \frac{\alpha}{n} \sum_{\substack{j=1 \\ j \neq i}}^n V_{ij}(\alpha n(z - \bar{x}_j)) - \frac{\alpha}{n} \sum_{\substack{j=1 \\ j \neq i}}^n V_{ij}(\alpha n(\bar{x}_i^- - \bar{x}_j)) < \frac{C}{n} \alpha V_{\text{eff}}\left(\frac{\alpha}{C}\right) - \frac{\alpha}{n} V(\alpha \bar{d}_n^-). \end{aligned}$$

Then, choosing α_0 large enough such that (91) applies, we obtain $\bar{d}_n^- \geq 1/(4C)$. We conclude that (95) holds.

Finally, we show that $\bar{x}^n \in \Omega_n^*$. By the singularity of V , it is enough to show that $\bar{d}_n^{+-} > r^*$. We reason by contradiction, and suppose that $\bar{d}_n^{+-} = r^*$. Treating $y = \bar{x}_1^-$ as a variable, we compute

$$\frac{d}{dy} \Big|_{y=\bar{x}_1^-} E_n(\bar{x}^n) = \frac{\alpha_n^2}{n^2} \sum_{i=2}^{n^-} -V'(\alpha_n(\bar{x}_i^- - \bar{x}_1^-)) - \frac{\alpha_n^2}{n^2} \sum_{i=1}^{n^+} -W'(\alpha_n(\bar{x}_1^- - \bar{x}_i^+)). \quad (96)$$

We show that the right-hand side of (96) is negative, which contradicts the minimality of $\bar{x}^n \in \bar{\Omega}_n^*$. Noting that $(-V'), (-W') > 0$ on $(0, \infty)$ and $(-V')$ is decreasing on $(0, \infty)$, we use (95) to estimate

$$\begin{aligned} \sum_{i=2}^{n^-} -V'(\alpha_n(\bar{x}_i^- - \bar{x}_1^-)) - \sum_{i=1}^{n^+} -W'(\alpha_n(\bar{x}_1^- - \bar{x}_i^+)) & < \left[\sum_{k=1}^{\infty} -V'(\alpha \bar{d}_n^- k) \right] - (-W')(\bar{d}_n^{+-}) \\ & < \left[\sum_{k=1}^{\infty} -V'(\alpha c k) \right] - |W'(r^*)|. \quad (97) \end{aligned}$$

Since $-V' \in L^1(1, \infty)$ is decreasing, the right-hand side of (97) is negative for all α large enough. For any such α , the right-hand side of (96) is negative too. The contradiction is reached, and we conclude that $\bar{x}^n \in \Omega_n^*$. \square

We reflect back on the numerical results in Table 5 with $\alpha = 2$. For the proof of Proposition 7.2 to apply to $\alpha = 2$, it is sufficient to derive a similar estimate as (97). Table 5 suggests that

$$\bar{d}_n^- := \min_{1 \leq i \leq n^-/2} n(\bar{x}_{i+1}^- - \bar{x}_i^-) > 0.99 \quad \text{for all } n^- \geq 8. \quad (98)$$

We choose a slightly different definition of \bar{d}_n^- then in (95) to avoid boundary-layer effects at the barrier at 1. Then, we redo the estimate in (97) to find

$$\sum_{k=1}^{\infty} |V'(\alpha \bar{d}_n^- k)| \approx \sum_{k=1}^{\infty} |V'(1.98k)| \approx 0.1576 < 0.4477 \approx |W'(r^*)|.$$

Hence, given that the estimate in (98) holds, the right-hand side in (97) is negative, and thus E_n has a local minimiser which is fully separated.

Supplementary to Proposition 1.2, we expect from our simulations in §7.1 with $\alpha_n = \frac{1}{2}n$ that complete mixing (85) occurs when $\alpha > 0$ is small enough. However, due to dynamical effects and the lack of convexity, this statement is hard to prove.

7.3. No separation in continuum energy. Proposition 7.2 shows that the continuum analogue of Proposition 1.2 does *not* hold for *any* $\alpha > 0$.

Definition 7.1 (Metric slope). *Let (X, d) be a complete metric space, and $\phi : X \rightarrow (-\infty, \infty]$ with domain $D(\phi) := \{x \in X : \phi(x) < \infty\} \neq \emptyset$. The metric slope of ϕ (with respect to the metric d) is*

$$|\partial\phi|_d : D(\phi) \rightarrow [0, \infty], \quad |\partial\phi|_d(x) := \limsup_{y \rightarrow x} \frac{[E(x) - E(y)]_+}{d(x, y)}.$$

Proposition 7.2 (E not critical at ρ_{sep}). *In the scaling regime $\frac{1}{n}\alpha_n \rightarrow \alpha > 0$ it holds that $|\partial E|_{\mathbf{W}}(\rho_{\text{sep}}) = \infty$. Moreover, there is a finite speed curve in $(M_{1/2}([0, 1]), \mathbf{W})$ connecting the separated state ρ_{sep} to the mixed state $\rho_{\text{mix}} := (\frac{1}{2}\mathcal{L}_{(0,1)}, \frac{1}{2}\mathcal{L}_{(0,1)})$ along which E is strictly decreasing.*

Proof. We set

$$\rho_t := \mathcal{L}_{(0, \frac{1}{2}(1-t))} + \frac{1}{2}\mathcal{L}_{(\frac{1}{2}(1-t), \frac{1}{2}(1+t))}, \quad 0 \leq t \leq 1,$$

and note that the curve

$$\rho_t := (\rho_t, 1 - \rho_t) \in M_{1/2}([0, 1]), \quad \text{for all } 0 \leq t \leq 1$$

satisfies the end conditions $\rho_0 = \rho_{\text{sep}}$ and $\rho_1 = \rho_{\text{mix}}$. The energy along the curve ρ_t is given by

$$E(\rho_t) = (1-t)\psi(1, 0) + t\psi(\frac{1}{2}, \frac{1}{2}).$$

Since $V > W$, it follows easily that the inequality in Lemma 4.10.(iii) is strict, and thus

$$\frac{d}{dt}E(\rho_t) = \psi(\frac{1}{2}, \frac{1}{2}) - \psi(1, 0) < 0.$$

We claim that

$$\mathbf{W}(\rho_t, \rho_s) = \frac{1}{2}\sqrt{\frac{t+2s}{3}}(t-s), \quad 0 \leq s \leq t \leq 1. \quad (99)$$

This claim implies Proposition 7.2, because it shows that ρ_t is a finite speed curve in $(M_{1/2}([0, 1]), \mathbf{W})$ connecting ρ_{sep} to ρ_{mix} , and

$$|\partial E|_{\mathbf{W}}(\rho_{\text{sep}}) = \limsup_{\mu \rightarrow \rho_{\text{sep}}} \frac{[E(\rho_{\text{sep}}) - E(\mu)]_+}{\mathbf{W}(\rho_{\text{sep}}, \mu)} \geq \limsup_{t \downarrow 0} \frac{[E(\rho_0) - E(\rho_t)]_+}{\mathbf{W}(\rho_0, \rho_t)} = \infty.$$

It remains to prove the claim (99). By the symmetry in ρ_t and $1 - \rho_t$, we obtain

$$\mathbf{W}^2(\rho_t, \rho_s) = \frac{1}{2}W^2(2\rho_t, 2\rho_s) + \frac{1}{2}W^2(2(1 - \rho_t), 2(1 - \rho_s)) = W^2(2\rho_t, 2\rho_s).$$

We observe that

$$X_t(\xi) := \begin{cases} \frac{1}{2}\xi & 0 < \xi < 1-t \\ \xi - \frac{1}{2}(1-t) & 1-t < \xi < 1 \end{cases}$$

is the inverse of the cumulative distribution of $2\rho_t$, i.e., $(X_t^{-1})' = 2\rho_t$. We use [Vil03, Thm. 2.18] to rewrite

$$W^2(2\rho_t, 2\rho_s) = \int_0^1 |X_t(\xi) - X_s(\xi)|^2 d\xi.$$

We continue to compute $W^2(2\rho_t, 2\rho_s)$ by

$$\begin{aligned} \int_0^1 |X_t(\xi) - X_s(\xi)|^2 d\xi &= \int_{1-t}^{1-s} \frac{1}{4} (\xi - (1-t))^2 d\xi + \int_{1-s}^1 \frac{1}{4} (t-s)^2 d\xi \\ &= \frac{1}{4} \int_0^{t-s} \eta^2 d\eta + \frac{s}{4} (t-s)^2 = \frac{t+2s}{12} (t-s)^2. \quad \square \end{aligned}$$

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APPENDIX A. PROPERTIES OF V (11) AND W (12)

In this section we prove Proposition 2.1 and (91).

Proof of Proposition 2.1. We compute

$$W'_a(r) = -2r \frac{1+a \cosh(2r)}{(\cosh(2r)+a)^2}, \quad W''_a(r) = 4r \sinh(2r) \frac{a \cosh(2r) + 2 - a^2}{(\cosh(2r)+a)^3} - 2 \frac{1+a \cosh(2r)}{(\cosh(2r)+a)^2}.$$

In particular, for V and $a \in \{0, 1\}$, we use the doubling formula's to simplify

$$\begin{aligned} V'(r) &= -\frac{r}{\sinh^2 r}, \quad W'_1(r) = -\frac{r}{\cosh^2 r} = W'_0\left(\frac{r}{2}\right), \\ V''(r) &= \frac{2r \coth r - 1}{\sinh^2 r}. \end{aligned} \quad (100)$$

Next we prove (i). Using that $\cosh(2r) + a \geq 1 + a > 0$, we can write W_a as a composition of smooth functions. Hence, W_a is smooth. Exponential decay of the tails of W_a is shown in [thesis, Prop. A.3.1]. The proof relies on basic Taylor expansions.

We continue with proving (ii). The ordering of the potentials W_a in a follows from

$$\frac{d}{da} W_a(r) = \frac{\frac{1}{2}}{\cosh(2r) + a} + \frac{r \sinh(2r)}{(\cosh(2r) + a)^2} > 0.$$

Since $W_a(r) \rightarrow 0$ as $r \rightarrow \infty$, we conclude $0 < W_0$ from (100) and $W_1 < V$ from $W'_1 > V'$ (100).

Next we prove (iii). Writing $\cosh(2r) = 2 \sinh^2 r + 1$, a straight-forward computation yields

$$\begin{aligned} &(V''(r) - W''_a(r)) (\cosh(2r) + a)^3 \sinh^2 r \\ &= (\cosh(2r) + a) (4(1-a) \sinh^4 r + (1+a)^2) (2r \coth r - 1) \\ &\quad + 4(1+a) (4ar \coth r - 1) \sinh^4 r + 2(1+a)^2 (4r \coth r - 1) \sinh^2 r. \end{aligned} \quad (101)$$

Except for $(4ar \coth r - 1)$, it follows from $\inf_{r>0} r \coth r = 1$ that all three terms in the right-hand side of (101) are non-negative for all $r \in \mathbb{R}$ and all $0 \leq a \leq 1$. We transfer a part of the first term to the second term such that both terms are non-negative. To this aim, we estimate the first term from below by

$$\begin{aligned} &(\cosh(2r) + a) (4(1-a) \sinh^4 r + (1+a)^2) (2r \coth r - 1) \\ &\geq (\cosh(2r) + a) (4(1-a) \sinh^4 r + (1+a)^2) (r \coth r - 1) + 4(1+a)(1-a)r \coth r \sinh^4 r. \end{aligned}$$

Using this estimate in (101), we obtain

$$\begin{aligned} & (V''(r) - W_a''(r))(\cosh(2r) + a)^3 \sinh^2 r \\ & \geq (\cosh(2r) + a)(4(1-a)\sinh^4 r + (1+a)^2)(r \coth r - 1) \\ & \quad + 4(1+a)((1+3a)r \coth r - 1)\sinh^4 r + 2(1+a)^2(4r \coth r - 1)\sinh^2 r, \end{aligned}$$

and observe that all terms are positive for all $0 \leq a \leq 1$ and all $r > 0$. Hence, $(V - W_a)'' > 0$ on $(0, \infty)$ for all $0 \leq a \leq 1$.

Finally, we prove (iv) by computing \widehat{W}_a explicitly. First, we focus on $0 \leq a < 1$. We use several common Fourier calculus relations to decompose \widehat{W}_a in several functions to which we can apply [Erdélyi I §1.9 (6)]:

$$\mathcal{F}\left(\frac{1}{\cosh(2r) + a}\right)(\omega) = \frac{\pi}{\sqrt{1-a^2}} \frac{\sinh(\pi \arccos(a)\omega)}{\sinh(\pi^2 \omega)} > 0.$$

We compute

$$\begin{aligned} \widehat{W}_a(r) &= \frac{1}{2\pi^2 \omega} \left[\mathcal{F}\left(\frac{W_a'(r)}{2r}\right) \right]' = \frac{-1}{2\pi^2 \omega} \left[\mathcal{F}\left(\frac{a}{\cosh(2r) + a} + \frac{1-a^2}{(\cosh(2r) + a)^2}\right) \right]' \\ &= \frac{-1}{2\pi \omega} \frac{a}{\sqrt{1-a^2}} \frac{d}{d\omega} \left(\frac{\sinh(\alpha\omega)}{\sinh(\beta\omega)} \right) - \frac{1}{2\omega} \frac{d}{d\omega} \left(\frac{\sinh(\alpha\omega)}{\sinh(\beta\omega)} \right) * \left(\frac{\sinh(\alpha\omega)}{\sinh(\beta\omega)} \right), \end{aligned} \quad (102)$$

where $\alpha := \pi \arccos(a) < \pi^2 =: \beta$. Since $f(\omega) := \sinh(\alpha\omega)/\sinh(\beta\omega)$ is even, it is sufficient to show that both terms in the right-hand side of (102) are positive for $\omega > 0$. To this aim, we compute

$$\begin{aligned} f'(\omega) &= \frac{\sinh(\beta\omega) \alpha \cosh(\alpha\omega) - \sinh(\alpha\omega) \beta \cosh(\beta\omega)}{\sinh^2(\beta\omega)} \\ &= \alpha \frac{\cosh(\alpha\omega)}{\sinh(\beta\omega)} \left(1 - \frac{\tanh(\alpha\omega)/(\alpha\omega)}{\tanh(\beta\omega)/(\beta\omega)} \right), \end{aligned}$$

which is negative for $\omega > 0$, since $\alpha < \beta$ and $x \mapsto \tanh(x)/x$ is decreasing on $(0, \infty)$. Hence, the first term in the right-hand side of (102) yields a positive contribution. Since f is moreover integrable, it holds that $f * f$ is decreasing on $(0, \infty)$, from which we infer positivity of the second term in the right-hand side of (102).

The case $a = 1$ simply follows from (100):

$$\widehat{W}_1(r) = 2\widehat{W}_0\left(\frac{r}{2}\right) = \widehat{W}_0\left(\frac{\omega}{2}\right) > 0. \quad \square$$

Proof of (91). We start by deriving a few estimates on V . [vM15, Prop. A.3.1] states that

$$V(r) = 2re^{-2r} + \mathcal{O}(re^{-4r}).$$

Hence, for all r large enough, we have $V(r) > \exp(-\frac{3}{2}r)$, and thus

$$V_{\text{eff}}(r) \leq \sum_{k=1}^{\infty} \exp(-\frac{3}{2}r)^k = \frac{\exp(-\frac{3}{2}r)}{1 - \exp(-\frac{3}{2}r)} \leq e^{-r} \quad \text{for all } r \text{ large enough.} \quad (103)$$

We also prove the following lower bound:

$$V(r) - e^{-2r} > 0 \quad \text{for all } r > 0. \quad (104)$$

Since $V(r) - e^{-2r} \rightarrow 0$ as $r \rightarrow \infty$, it is enough to show that $\frac{d}{dr}(V(r) - e^{-2r}) < 0$ on $(0, \infty)$. Recalling (100), we compute

$$\begin{aligned} \frac{d}{dr}(V(r) - e^{-2r}) &= -\frac{r}{\sinh^2 r} + 2e^{-2r} = \frac{2(1 - e^{-2r})^2 - 4r}{(e^r - e^{-r})^2} \\ &\leq \frac{2}{(e^r - e^{-r})^2} \left\{ \begin{array}{ll} (2r)^2 - 2r, & 0 < r < \frac{1}{2} \\ (1 - \frac{1}{e})^2 - 1, & r = \frac{1}{2} \\ 1 - 2r, & \frac{1}{2} < r \end{array} \right\} < 0. \end{aligned}$$

Next we prove (91). We fix any $C > 0$, set $\alpha_0 \geq 2C \log C$ such that (103) holds for all $r \geq \alpha_0/C$, and take any $0 < x < 1/(4C)$. Then, by (103) and (104) we have

$$\sup_{\alpha > \alpha_0} \left[CV_{\text{eff}}\left(\frac{\alpha}{C}\right) - V(\alpha x) \right] \leq \sup_{\alpha > \alpha_0} \underbrace{\left[\exp\left(\log C - \frac{\alpha}{C}\right) - \exp(-2\alpha x) \right]}_{\varphi(\alpha, x)}. \quad (105)$$

Since $x < 1/(2C)$, the second exponential in $\varphi(\alpha, x)$ decays slower as $\alpha \rightarrow \infty$ than the first exponential. In particular, if $C \leq 1$, then $\sup_{\alpha > 0} \varphi(\alpha) = 0$, and thus it suffices to assume $C > 1$. For $C > 1$, we note that the equation $\varphi(\alpha, x) = 0$ has a unique solution α^x , which is given by

$$\alpha^x := \frac{C \log C}{1 - 2Cx} < 2C \log C \leq \alpha_0.$$

Moreover, $\sup_{\alpha > \alpha^x} \varphi(\alpha, x) = 0$. Hence, if we further assume $x < 1/(4C)$, then $\alpha^x \leq 2C \log C \leq \alpha_0$, and thus

$$0 = \sup_{\alpha > \alpha^x} \varphi(\alpha, x) \geq \sup_{\alpha > \alpha_0} \varphi(\alpha, x).$$

Together with (105), we conclude (91). \square

APPENDIX B. PROOF OF LEMMA 6.3

Proof of Lemma 6.3. The symmetry property stated in Lemma 6.3.(i) follows directly from the definition. We continue by showing that \mathbf{W} as defined in (73) is a metric. Symmetry, non-negativity and the property that $\mathbf{W}(\boldsymbol{\mu}, \boldsymbol{\nu}) = 0$ implies $\boldsymbol{\mu} = \boldsymbol{\nu}$ are easily checked. To prove the triangle inequality, we consider arbitrary $\boldsymbol{\mu}_i \in M([0, 1])$ for $i = 1, 2, 3$, and let $\boldsymbol{\sigma}_i := \boldsymbol{\mu}_i([0, 1])$ the corresponding masses. For convenience, we set

$$\mathbf{w}_{ij} := \mathbf{W}^2(\boldsymbol{\mu}_i, \boldsymbol{\mu}_j), \quad w_{ij}^\pm := W^2\left(\frac{\mu_i^\pm}{\sigma_i^\pm}, \frac{\mu_j^\pm}{\sigma_j^\pm}\right), \quad \sigma_{ij}^\pm := \sigma_i^\pm \wedge \sigma_j^\pm, \quad d_{ij}^\pm := |\sigma_i^\pm - \sigma_j^\pm|$$

for all $1 \leq i < j \leq 3$, and set $\sum_{p=\pm} \beta^p := \beta^+ + \beta^-$ for any symbol β . We prove the triangle inequality in squared form:

$$\mathbf{w}_{12} + \mathbf{w}_{23} + 2\sqrt{\mathbf{w}_{12}\mathbf{w}_{23}} - \mathbf{w}_{13} \geq 0. \quad (106)$$

We start with a few observations. (73) reads

$$\mathbf{w}_{ij} = \sum_{p=\pm} (\sigma_{ij}^p w_{ij}^p + d_{ij}^p).$$

Since W satisfies the triangle inequality, we have

$$w_{13}^\pm \leq w_{12}^\pm + w_{23}^\pm + 2\sqrt{w_{12}^\pm w_{23}^\pm}. \quad (107)$$

For the constants σ_{ij}^\pm and d_{ij}^\pm , it holds that

$$\sigma_{ij}^\pm + d_{ij}^\pm = \sigma_i^\pm \vee \sigma_j^\pm \geq \sigma_{13}^\pm \quad \text{for all } 1 \leq i < j \leq 3. \quad (108)$$

Finally, for $p \in \{+, -\}$,

$$\sigma_2^p \geq \sigma_{13}^p \implies \sigma_{12}^p \wedge \sigma_{23}^p = \sigma_{13}^p \text{ and } d_{12}^p + d_{23}^p \geq d_{13}^p, \quad (109)$$

and,

$$\sigma_2^p < \sigma_{13}^p \implies \begin{cases} \sigma_2^p - \sigma_{13}^p + d_{12}^p = 0 \text{ and } d_{12}^p + d_{23}^p = 2d_{12}^p + d_{13}^p, & \text{if } \sigma_1^p \leq \sigma_3^p, \\ \sigma_2^p - \sigma_{13}^p + d_{23}^p = 0 \text{ and } d_{12}^p + d_{23}^p = 2d_{23}^p + d_{13}^p, & \text{if } \sigma_3^p \leq \sigma_1^p. \end{cases} \quad (110)$$

Next we prove (106). Using (107), we estimate

$$\mathbf{w}_{13} = \sum_{p=\pm} (\sigma_{13}^p w_{13}^p + d_{13}^p) \leq \sum_{p=\pm} (\sigma_{13}^p w_{12}^p + \sigma_{13}^p w_{23}^p + 2\sigma_{13}^p \sqrt{w_{12}^p w_{23}^p} + d_{13}^p),$$

and find

$$\begin{aligned} \mathbf{w}_{12} + \mathbf{w}_{23} + 2\sqrt{\mathbf{w}_{12}\mathbf{w}_{23}} - \mathbf{w}_{13} &\geq \sum_{p=\pm} \left[(\sigma_{12}^p - \sigma_{13}^p)w_{12}^p + (\sigma_{23}^p - \sigma_{13}^p)w_{23}^p + d_{12}^p + d_{23}^p - d_{13}^p \right] \\ &\quad + 2 \left[\sqrt{\sum_{p=\pm} \sum_{q=\pm} (\sigma_{12}^p w_{12}^p + d_{12}^p)(\sigma_{23}^q w_{23}^q + d_{23}^q)} - \sum_{p=\pm} \sigma_{13}^p \sqrt{w_{12}^p w_{23}^p} \right]. \end{aligned}$$

It is enough to prove that both terms in the right-hand side are non-negative. Non-negativity of the first term follow either from (109) or from (110) with $w_{ij}^p \leq 1$. To prove non-negativity of the second term, we show that the first term within brackets is larger or equal to the second term by using respectively $w_{ij}^p \leq 1$, (108) and $a + b \geq 2\sqrt{ab}$, i.e.,

$$\begin{aligned} \sum_{p=\pm} \sum_{q=\pm} (\sigma_{12}^p w_{12}^p + d_{12}^p)(\sigma_{23}^q w_{23}^q + d_{23}^q) &\geq \sum_{p=\pm} \sum_{q=\pm} (\sigma_{12}^p + d_{12}^p)w_{12}^p (\sigma_{23}^q + d_{23}^q)w_{23}^q \\ &\geq \sum_{p=\pm} \sum_{q=\pm} \sigma_{13}^p w_{12}^p \sigma_{13}^q w_{23}^q = \sum_{p=\pm} \sigma_{13}^p w_{12}^p \sigma_{13}^p w_{23}^p + \sum_{p=\pm} \sigma_{13}^p \sigma_{13}^{-p} w_{12}^p w_{23}^{-p} \\ &\geq \sum_{p=\pm} \sigma_{13}^p \sigma_{13}^p w_{12}^p w_{23}^p + 2\sigma_{13}^+ \sigma_{13}^- \sqrt{w_{12}^+ w_{23}^- w_{12}^- w_{23}^+} = \sum_{p=\pm} \sum_{q=\pm} \sigma_{13}^p \sigma_{13}^q \sqrt{w_{12}^p w_{23}^p w_{12}^q w_{23}^q} \\ &= \left(\sum_{p=\pm} \sigma_{13}^p \sqrt{w_{12}^p w_{23}^p} \right)^2. \end{aligned}$$

This completes the proof for \mathbf{W} satisfying the triangle inequality, which is the last step for proving that \mathbf{W} is a metric.

Separability follows easily from $(P([0, 1]), W)$ being separable. We continue with proving completeness. Let (μ_k) be a \mathbf{W} -Cauchy sequence with masses $\sigma_k := \mu_k([0, 1])$. From the definition of \mathbf{W} in (73) it follows that σ_k^\pm are Cauchy sequences in $[0, 1]$, which therefore converge to the limiting values $\sigma^\pm \in [0, 1]$, which moreover satisfy $\sigma^+ + \sigma^- = 1$.

Let us first consider the case in which $\sigma^+ \in (0, 1)$. Then, for all k large enough, $\sigma_k^\pm \geq \frac{1}{2}\sigma^\pm > 0$. It follows from the definition of \mathbf{W} that μ_k^\pm/σ_k^\pm are W -Cauchy sequences in $\mathcal{P}([0, 1])$, and hence (μ_k^\pm/σ_k^\pm) converges to some $\tilde{\mu}^\pm \in \mathcal{P}([0, 1])$ with respect to W . Setting $\mu^\pm := \sigma^\pm \tilde{\mu}^\pm$, we conclude that $\mathbf{W}(\mu_k, \mu) \rightarrow 0$ as $k \rightarrow \infty$.

The final step of the proof for completeness is to treat the case $\sigma^+ \in \{0, 1\}$. By symmetry between the positive and the negative parts, it is enough to consider $\sigma^+ = 0$. By the previous argument, we obtain that μ_k^-/σ_k^- converges to $\mu^- \in \mathcal{P}([0, 1])$ with respect to W . Consequently, we need to set $\mu^+ = 0$ in order for $\mu \in M([0, 1])$. we find from (74) that

$$\mathbf{W}^2(\mu_k, \mu) = \sigma_k^+ + \sigma_k^- W^2\left(\frac{\mu_k^-}{\sigma_k^-}, \mu^-\right) + |\sigma_k^- - 1| \xrightarrow{k \rightarrow \infty} 0.$$

Next we prove the equivalence between the topology induced by \mathbf{W} and the narrow topology as in Lemma 6.3.(ii). We show that this is a consequence of [AGS08, Prop. 7.1.5], which states that for $(\mu_k) \subset \mathcal{P}([0, 1])$,

$$\mu_k \rightharpoonup \mu \iff W(\mu_k, \mu) \rightarrow 0. \quad (111)$$

We first prove that $\mu_k \rightharpoonup \mu$ implies $\mathbf{W}(\mu_k, \mu) \rightarrow 0$. Choosing $\varphi^\pm \equiv 1$ in (4), we find that the masses satisfy $\sigma_k^\pm \rightarrow \sigma^\pm$. By Lemma 6.3.(i), it is therefore enough to show that

$$(\sigma_k^+ \wedge \sigma^+) W^2\left(\frac{\mu_k^+}{\sigma_k^+}, \frac{\mu^+}{\sigma^+}\right) \rightarrow 0. \quad (112)$$

This is trivial for $\sigma^+ = 0$, so let us assume $\sigma^+ > 0$. We take k large enough such that $\sigma_k^+ > \sigma^+/2 > 0$. Then, $(\sigma_k^+)^{-1} \rightarrow (\sigma^+)^{-1}$, and thus

$$\frac{\mu_k^+}{\sigma_k^+} \rightharpoonup \frac{\mu^+}{\sigma^+}. \quad (113)$$

We conclude from (111) that (112) holds.

Next we prove the opposite implication. Let $\mathbf{W}(\mu_k, \mu) \rightarrow 0$. Again, $\sigma_k^\pm \rightarrow \sigma^\pm$, and by Lemma 6.3.(i) it is enough to show $\mu_k^+ \rightharpoonup \mu^+$. If $\sigma^+ = 0$, then $\mu^+ = 0$ and $\sigma_k^+ \rightarrow 0$, and thus

$$\left| \int \varphi d\mu_k^+ \right| \leq \sigma_k^+ \|\varphi\|_\infty \xrightarrow{k \rightarrow \infty} 0 = \int \varphi d\mu^+$$

for any test function $\varphi \in C([0, 1])$. If $\sigma^+ > 0$, then we take k large enough such that $\sigma_k^+ > \sigma^+/2 > 0$. Then, $\mathbf{W}(\mu_k, \mu) \rightarrow 0$ implies

$$W^2\left(\frac{\mu_k^+}{\sigma_k^+}, \frac{\mu^+}{\sigma^+}\right) \rightarrow 0.$$

By (111) we obtain (113), and we conclude $\mu_k^+ \rightharpoonup \mu^+$ from $(\sigma_k^+)^{-1} \rightarrow (\sigma^+)^{-1}$.

With Lemma 6.3.(ii) established, sequential compactness follows from Prokhorov, which states that any sequence μ_k has a narrowly converging subsequence.

Next we prove that $M_{\sigma^+}([0, 1])$ is non-positively curved (see (70)), i.e., for all $\mu_0, \mu_1, \nu \in M_{\sigma^+}([0, 1])$,

$$\mathbf{W}^2(\mu_t, \nu) \leq (1-t)\mathbf{W}^2(\mu_0, \nu) + t\mathbf{W}^2(\mu_1, \nu) - t(1-t)\mathbf{W}^2(\mu_0, \mu_1) \quad \text{for all } 0 \leq t \leq 1, \quad (114)$$

where μ_t is a geodesic connecting μ_0 and μ_1 . Since the case $\sigma^+ \in \{0, 1\}$ follows by a simplification of the argument below, we assume $\sigma^+ \in (0, 1)$. To characterise μ_t , let $\tilde{\mu}_t^\pm$ be a W -geodesic in $\mathcal{P}([0, 1])$ connecting μ_0^\pm/σ^\pm with μ_1^\pm/σ^\pm . We observe that $\mu_t := (\sigma^+ \tilde{\mu}_t^+, \sigma^- \tilde{\mu}_t^-) \in M_{\sigma^+}([0, 1])$ is a \mathbf{W} -geodesic (see (69)) from

$$\mathbf{W}^2(\mu_s, \mu_t) = \sum_{p=\pm} \frac{1}{\sigma^p} W^2(\tilde{\mu}_s^\pm, \tilde{\mu}_t^\pm) = \sum_{p=\pm} \frac{1}{\sigma^p} (t-s)^2 W^2(\tilde{\mu}_0^\pm, \tilde{\mu}_1^\pm) = (t-s)^2 \mathbf{W}^2(\mu_0, \mu_1),$$

which holds for all $0 \leq s \leq t \leq 1$. Then, by the additive structure of \mathbf{W} as in (75) which separates the dependence on μ^+ and μ^- , (114) follows directly from $(\mathcal{P}([0, 1]), W)$ being non-positively curved (which is a consequence of [AGS08, (7.2.8)]).

Next we prove the characterisation in Lemma 6.3.(iii) of $\mathbf{W}^2(\mu_n, \nu_n)$ for the empirical measures μ_n and ν_n corresponding to $x^n, y^n \in \Omega_n$. For any such measures, we compute

$$\begin{aligned} \mathbf{W}^2(\mu_n, \nu_n) &= \frac{n^+}{n} W^2\left(\frac{1}{n^+} \sum_{i=1}^{n^+} \delta_{x_i^+}, \frac{1}{n^+} \sum_{i=1}^{n^+} \delta_{y_i^+}\right) + \frac{n^-}{n} W^2\left(\frac{1}{n^-} \sum_{i=1}^{n^-} \delta_{x_i^-}, \frac{1}{n^-} \sum_{i=1}^{n^-} \delta_{y_i^-}\right) \\ &= \frac{n^+}{n} \frac{1}{n^+} \sum_{i=1}^{n^+} (x_i^+ - y_i^+)^2 + \frac{n^-}{n} \frac{1}{n^-} \sum_{i=1}^{n^-} (x_i^- - y_i^-)^2 = \frac{1}{n} |x^n - y^n|^2. \end{aligned} \quad (115)$$

Finally, we prove the property of geodesics in $M([0, 1])$ stated in Lemma 6.3.(iv). We reason by contradiction. Let $t \mapsto \mu_t$ be any \mathbf{W} -geodesic for which there exists a $t \in (0, 1)$ such that $\mu_t \notin M_{\sigma^+}([0, 1])$. Setting $\sigma_t^\pm := \mu_t^\pm([0, 1])$, we define $\nu^\pm := \sigma^\pm \mu_t^\pm / \sigma_t^\pm$, and note that $\nu \in M_\sigma([0, 1])$. We compute

$$\mathbf{W}^2(\mu_0, \mu_t) = \mathbf{W}^2(\mu_0, \nu) + \mathbf{W}^2(\nu, \mu_t) > \mathbf{W}^2(\mu_0, \nu),$$

and, similarly, $\mathbf{W}(\mu_1, \mu_t) > \mathbf{W}(\mu_1, \nu)$. Hence, $t \mapsto \mu_t$ is not a geodesic. \square

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